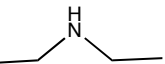
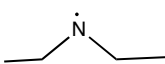


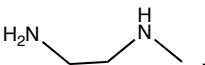
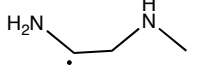
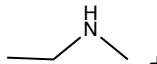
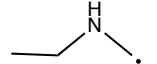
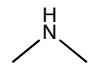
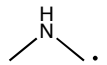
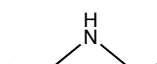
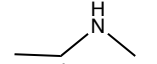
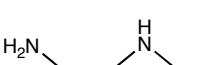
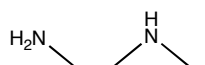


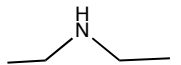
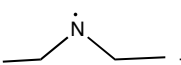
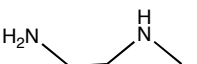
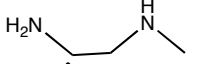


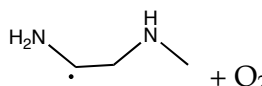
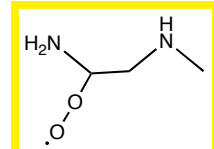
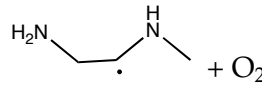
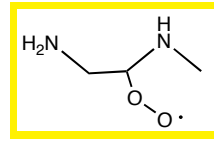
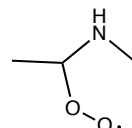
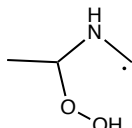
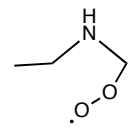
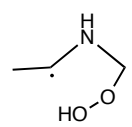
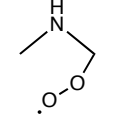
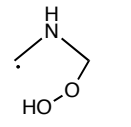
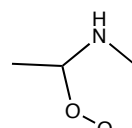
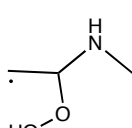
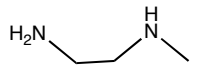
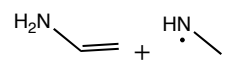
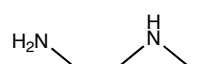
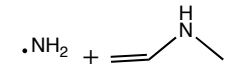
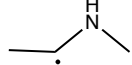
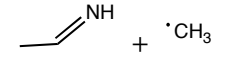
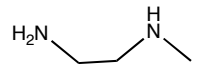
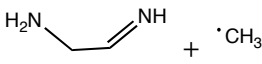
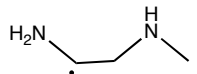
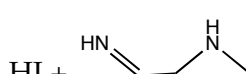
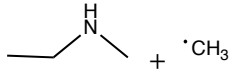
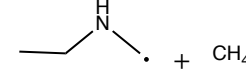
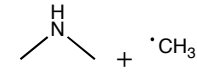
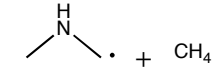
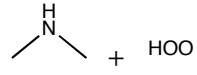
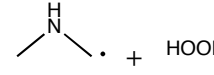
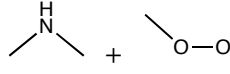
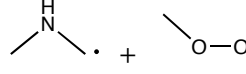
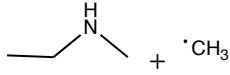
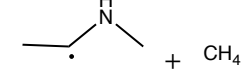
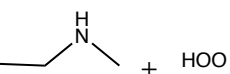
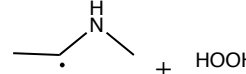
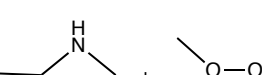
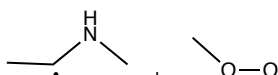
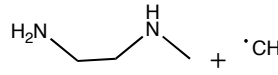
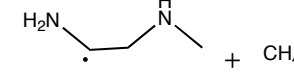
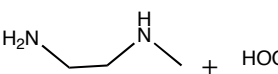
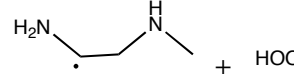
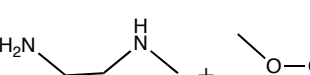
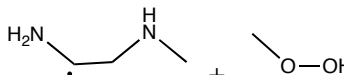
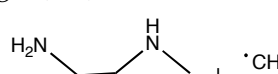
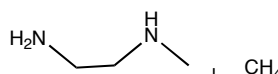


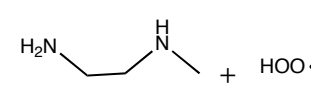
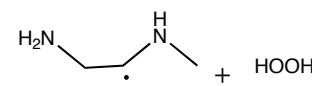
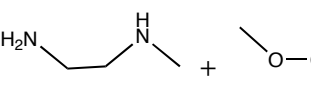
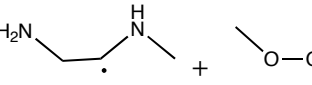
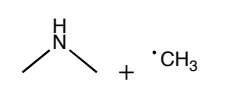
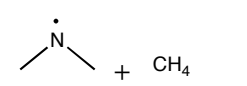
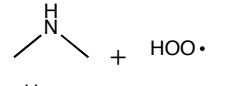
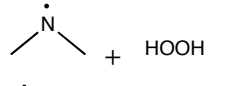
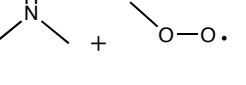
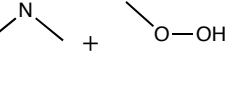
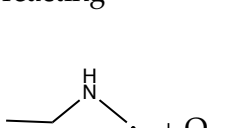
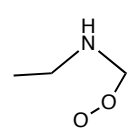
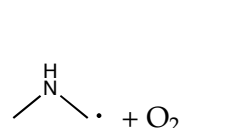
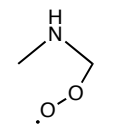
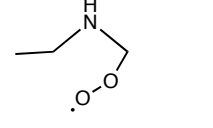
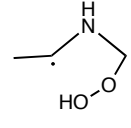
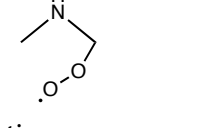
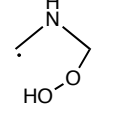
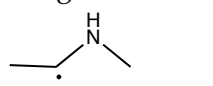
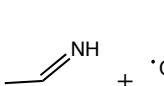
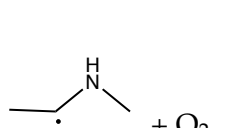
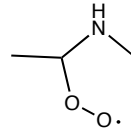
Table 1: CBS-QB3 Energies

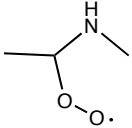
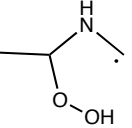
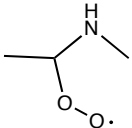
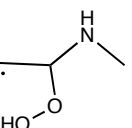
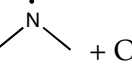
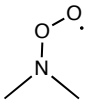
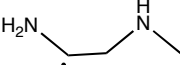
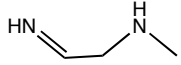
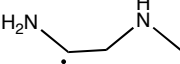
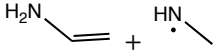
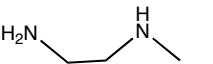
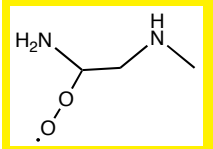
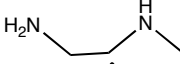
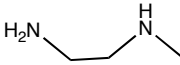
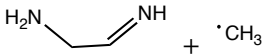
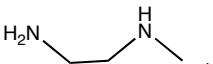
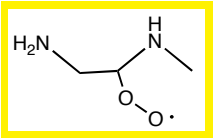


	reactants	$\rightleftharpoons$	products	$\Delta E_{\text{rxn}}$ (kcal/mol)	barrier
23	$\text{HOO}\cdot + \text{HOO}\cdot$	$\rightleftharpoons$	$\text{HOOH} + \text{O}_2$	-38.5	—
That was a test. According to 10.1021/jp066823d it has a ZPVE-corrected CASPT2/6-311+G(3df,2p) total energy change of -39.5 kcal/mol					
Grouped the new way					
Making radical from $\cdot\text{CH}_3$					
24	 + $\cdot\text{CH}_3$	$\rightleftharpoons$	 + $\text{CH}_4$	-11.1	—
12	 + $\cdot\text{CH}_3$	$\rightleftharpoons$	 + $\text{CH}_4$	-11.2	8.1 8.1
25	 + $\cdot\text{CH}_3$	$\rightleftharpoons$	 + $\text{CH}_4$	-11.6	—
3	 + $\cdot\text{CH}_3$	$\rightleftharpoons$	 + $\text{CH}_4$	-12.3	10.1 10.1
11	 + $\cdot\text{CH}_3$	$\rightleftharpoons$	 + $\text{CH}_4$	-12.4	10.2 10.2
4	 + $\cdot\text{CH}_3$	$\rightleftharpoons$	 + $\text{CH}_4$	-13.5	8.4 8.4
26	 + $\cdot\text{CH}_3$	$\rightleftharpoons$	 + $\text{CH}_4$	-14.4	—
Making radical from $\text{HOO}\cdot$					
16	 + $\text{HOO}\cdot$	$\rightleftharpoons$	 + $\text{HOOH}$	6.1	9.0 2.9
1	 + $\text{HOO}\cdot$	$\rightleftharpoons$	 + $\text{HOOH}$	6.2	7.0 0.8
27	 + $\text{HOO}\cdot$	$\rightleftharpoons$	 + $\text{HOOH}$	5.7	—
15	 + $\text{HOO}\cdot$	$\rightleftharpoons$	 + $\text{HOOH}$	4.8	7.6 2.7


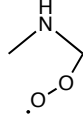
CBS-QB3 Energies (kcal/mol)				$\Delta E_{\text{rxn}}$	barrier	
6				3.7	5.7	2.0
28				2.8	—	
Making radical from CH <sub>3</sub> OO•						
14				7.6	9.7	2.1
29				7.2	—	
13				6.3	8.2	1.8
5				5.2	6.4	1.1
30				4.3	—	
O <sub>2</sub> addition to radical						
31				−6.9	—	
32				−31.8	—	
33				−32.0	—	
34				−32.4	—	

CBS-QB3 Energies (kcal/mol)				$\Delta E_{\text{rxn}}$	barrier	
35	 $+ \text{O}_2 \rightleftharpoons$		—	—		
36	 $+ \text{O}_2 \rightleftharpoons$		—	—		
Intramolecular H-abstraction						
9	 $\rightleftharpoons$		5.0	13.2	8.2	
2	 $\rightleftharpoons$		7.3	14.1	6.8	
10	 $\rightleftharpoons$		8.4	15.9	7.5	
8	 $\rightleftharpoons$		18.5	32.5	14.0	
$\beta$ -scission of a radical						
20	 $\rightleftharpoons$		17.9	21.8	3.9	
18	 $\rightleftharpoons$		24.0	26.0	2.0	
7	 $\rightleftharpoons$		16.1	28.1	11.9	
17	 $\rightleftharpoons$		18.0	29.9	11.9	

CBS-QB3 Energies (kcal/mol)				$\Delta E_{\text{rxn}}$	barrier	
19		$\rightleftharpoons$		34.7	37.5	2.8
Grouped by radical type						
Making C1 radical						
3		$\rightleftharpoons$		-12.3	10.1	10.1
11		$\rightleftharpoons$		-12.4	10.2	10.2
15		$\rightleftharpoons$		4.8	7.6	2.7
13		$\rightleftharpoons$		6.3	8.2	1.8
Making C2 radical						
4		$\rightleftharpoons$		-13.5	8.4	8.4
6		$\rightleftharpoons$		3.7	5.7	2.0
5		$\rightleftharpoons$		5.2	6.4	1.1
Making C(N1) radical						
25		$\rightleftharpoons$		-11.6	—	—
27		$\rightleftharpoons$		5.7	—	—
29		$\rightleftharpoons$		7.2	—	—
Making C(N2) radical						
26		$\rightleftharpoons$		-14.4	—	—

CBS-QB3 Energies (kcal/mol)				$\Delta E_{\text{rxn}}$	barrier	
28		$\rightleftharpoons$		2.8	—	
30		$\rightleftharpoons$		4.3	—	
Making N radical						
12		$\rightleftharpoons$		-11.2	8.1	8.1
16		$\rightleftharpoons$		6.1	9.0	2.9
14		$\rightleftharpoons$		7.6	9.7	2.1
C1 radical reacting						
33		$\rightleftharpoons$		-32.0	—	
32		$\rightleftharpoons$		-31.8	—	
2		$\rightleftharpoons$		7.3	14.1	6.8
10		$\rightleftharpoons$		8.4	15.9	7.5
C2 radical reacting						
7		$\rightleftharpoons$		16.1	28.1	11.9
34		$\rightleftharpoons$		-32.4	—	

CBS-QB3 Energies (kcal/mol)				$\Delta E_{\text{rxn}}$	barrier	
9		$\rightleftharpoons$		5.0	13.2	8.2
8		$\rightleftharpoons$		18.5	32.5	14.0
N radical reacting						
31		$+ \text{O}_2$	$\rightleftharpoons$		-6.9	—
C(N1) radical reacting						
19		$\rightleftharpoons$	HJ + 	34.7	37.5	2.8
20		$\rightleftharpoons$		17.9	21.8	3.9
35		$+ \text{O}_2$	$\rightleftharpoons$		—	—
C(N2) radical reacting						
18		$\rightleftharpoons$	$\cdot\text{NH}_2 + \text{CH}_2=\text{N}(\text{CH}_3)_2$	24.0	26.0	2.0
17		$\rightleftharpoons$		18.0	29.9	11.9
36		$+ \text{O}_2$	$\rightleftharpoons$		—	—
These are mistakes I might have made earlier:						
37		$+ \cdot\text{CH}_3 + \text{O}_2 \text{ singlet}$	$\rightleftharpoons$		-46.7	—

CBS-QB3 Energies (kcal/mol)				$\Delta E_{\text{rxn}}$	barrier
38	 <chem>CCNCC</chem>	$+ \cdot\text{CH}_3 + \text{O}_2\text{singlet} \rightleftharpoons$	 <chem>CCNCCOO</chem>	$+ \text{CH}_4$	$-73.0$ —