

How to Add a Five-Membered Ring to Polycyclic Aromatic Hydrocarbons (PAHs) – Molecular Mass Growth of the 2-Naphthyl Radical ($C_{10}H_7$) to Benzindenes ($C_{13}H_{10}$) as a Case Study

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Calculated product branching ratios of the 2-naphthyl + C₃H₄ reactions at various pressures and temperatures.

(a) 2-naphthyl + allene, 0.03 atm.

T, K	methyl-acetylene	p1	p2	p3	p4	p5	p6	p7	i1	i7	i14	i17	i18	3-ring total	2-ring total	stabilization
300	0.00%	0.01%	0.01%	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	17.85%	81.34%	0.23%	0.46%	0.03%	0.00%	99.88%
400	0.00%	0.12%	0.16%	0.16%	0.00%	0.00%	0.00%	0.00%	0.00%	36.48%	60.49%	0.86%	1.72%	0.43%	0.00%	99.56%
500	0.00%	0.83%	0.90%	0.88%	0.00%	0.01%	0.01%	0.00%	0.00%	61.78%	30.98%	2.40%	2.22%	2.61%	0.02%	97.37%
600	0.00%	2.62%	2.26%	2.23%	0.00%	0.03%	0.06%	0.00%	0.00%	78.79%	9.95%	2.17%	1.89%	7.11%	0.09%	92.80%
700	0.00%	4.75%	3.45%	3.39%	0.01%	0.09%	0.22%	0.02%	0.02%	83.75%	2.29%	1.19%	0.80%	11.59%	0.34%	88.05%
800	0.04%	6.50%	4.23%	4.16%	0.10%	0.22%	0.69%	0.18%	0.04%	82.67%	0.48%	0.43%	0.22%	14.90%	1.20%	83.85%
900	0.18%	8.28%	5.09%	5.00%	0.37%	0.54%	1.97%	0.82%	0.06%	77.49%		0.12%	0.05%	18.37%	3.70%	77.72%
1000	0.55%	10.74%	6.41%	6.29%	0.91%	1.20%	4.89%	2.38%	0.09%	66.50%		0.03%	0.01%	23.43%	9.38%	66.64%
1100	1.15%	13.68%	8.01%	7.85%	1.58%	2.25%	10.22%	4.92%	0.11%	50.22%		0.01%	0.00%	29.54%	18.96%	50.35%
1200	1.84%	15.94%	9.20%	9.02%	2.11%	3.58%	17.92%	7.74%		32.62%				34.16%	31.36%	32.62%
1300	2.38%	16.53%	9.44%	9.25%	2.23%	4.93%	26.97%	9.88%		18.38%				35.22%	44.01%	18.38%
1400	2.68%	15.53%	8.77%	8.59%	2.03%	6.08%	36.14%	10.92%		9.23%				32.89%	55.18%	9.23%
1500	2.78%	13.60%	7.61%	7.45%	1.69%	6.95%	44.60%	11.05%		4.26%				28.67%	64.28%	4.26%
1600	2.81%	11.81%	6.57%	6.42%	1.44%	7.65%	52.40%	10.91%						24.80%	72.39%	
1700	2.65%	9.51%	5.24%	5.12%	1.07%	8.00%	58.40%	10.01%						19.87%	77.48%	
1800	2.49%	7.64%	4.18%	4.08%	0.80%	8.22%	63.46%	9.12%						15.90%	81.61%	
1900	2.33%	6.15%	3.34%	3.27%	0.61%	8.34%	67.68%	8.29%						12.75%	84.92%	
2000	2.17%	4.97%	2.69%	2.62%	0.47%	8.38%	71.17%	7.53%						10.28%	87.55%	
2100	2.02%	4.04%	2.18%	2.13%	0.37%	8.38%	74.05%	6.84%						8.35%	89.63%	
2200	1.88%	3.32%	1.78%	1.74%	0.29%	8.33%	76.44%	6.22%						6.83%	91.29%	
2300	1.75%	2.74%	1.47%	1.43%	0.24%	8.26%	78.44%	5.67%						5.64%	92.61%	
2400	1.63%	2.29%	1.22%	1.19%	0.19%	8.18%	80.12%	5.18%						4.70%	93.67%	
2500	1.51%	1.93%	1.03%	1.00%	0.16%	8.09%	81.53%	4.75%						3.95%	94.53%	

(b) 2-naphthyl + allene, 1 atm.

T, K	methyl- acetylene	p1	p2	p3	p4	p5	p6	p7	i1	i7	i14	i17	i18	3-ring total	2-ring total	stabilization
300	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	11.64%	88.33%	0.00%	0.00%	0.00%	0.00%	99.97%
400	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	17.07%	82.80%	0.03%	0.05%	0.00%	0.00%	99.94%
500	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	23.52%	75.84%	0.18%	0.00%	0.01%	0.00%	99.55%
600	0.00%	0.05%	0.06%	0.06%	0.00%	0.01%	0.02%	0.00%	0.00%	33.98%	63.70%	0.85%	1.14%	0.18%	0.02%	99.67%
700	0.00%	0.35%	0.39%	0.39%	0.00%	0.04%	0.11%	0.00%	0.00%	49.54%	44.63%	2.02%	2.27%	1.13%	0.16%	98.46%
800	0.00%	1.31%	1.25%	1.23%	0.00%	0.14%	0.45%	0.00%	0.00%	64.68%	24.94%	3.05%	2.92%	3.79%	0.60%	95.59%
900	0.00%	3.01%	2.43%	2.39%	0.01%	0.33%	1.26%	0.03%	0.01%	73.75%	11.70%	2.83%	2.24%	7.83%	1.62%	90.53%
1000	0.03%	4.86%	3.41%	3.35%	0.03%	0.63%	2.78%	0.13%	0.02%	76.61%	5.00%	1.90%	1.23%	11.63%	3.57%	84.76%
1100	0.10%	6.41%	4.09%	4.01%	0.10%	1.10%	5.36%	0.44%	0.03%	76.60%		1.10%	0.63%	14.51%	6.98%	78.36%
1200	0.27%	7.41%	4.45%	4.36%	0.21%	1.76%	9.46%	1.15%	0.08%	70.10%		0.50%	0.24%	16.22%	12.58%	70.93%
1300	0.58%	8.17%	4.73%	4.64%	0.41%	2.67%	15.53%	2.38%		60.52%		0.23%	0.10%	17.54%	20.99%	60.85%
1400	1.00%	8.78%	4.95%	4.84%	0.58%	3.79%	23.64%	3.97%		48.40%				18.57%	31.97%	48.40%
1500	1.43%	8.84%	4.93%	4.83%	0.69%	4.99%	33.12%	5.56%		35.56%				18.60%	44.35%	35.56%
1600	1.78%	8.45%	4.67%	4.57%	0.72%	6.10%	42.84%	6.79%		23.99%				17.69%	56.44%	23.99%
1700	2.02%	7.67%	4.22%	4.12%	0.68%	6.98%	51.74%	7.49%		15.02%				16.01%	66.89%	15.02%
1800	2.12%	6.70%	3.66%	3.57%	0.61%	7.60%	59.21%	7.69%		8.79%				13.93%	75.11%	8.79%
1900	2.33%	6.20%	3.37%	3.29%	0.62%	8.33%	67.55%	8.30%						12.86%	84.82%	0.00%
2000	2.17%	4.99%	2.70%	2.64%	0.48%	8.38%	71.10%	7.54%						10.33%	87.50%	0.00%
2100	2.02%	4.05%	2.18%	2.13%	0.37%	8.37%	74.02%	6.84%						8.37%	89.61%	0.00%
2200	1.88%	3.32%	1.78%	1.74%	0.30%	8.33%	76.43%	6.22%						6.84%	91.28%	0.00%
2300	1.75%	2.75%	1.47%	1.43%	0.24%	8.26%	78.43%	5.67%						5.65%	92.61%	0.00%
2400	1.63%	2.29%	1.22%	1.19%	0.19%	8.18%	80.11%	5.18%						4.70%	93.67%	0.00%
2500	1.51%	1.93%	1.03%	1.00%	0.16%	8.09%	81.53%	4.75%						3.96%	94.53%	0.00%

(c) 2-naphthyl + allene, zero-pressure limit.

T, K	methyl-acetylene	p1	p2	p3	p4	p5	p6	p7	i1	i7	i14	i17	i18	3-ring total	2-ring total	stabilization
300	0.00%	27.84%	21.71%	21.37%	0.54%	0.06%	0.00%	0.22%		28.25%				70.92%	0.82%	28.25%
400	0.04%	36.17%	26.24%	25.97%	1.93%	0.22%	0.01%	0.92%		8.48%				88.39%	3.08%	8.48%
500	0.20%	38.21%	26.67%	26.35%	4.15%	0.50%	0.08%	2.31%		1.52%				91.23%	7.05%	1.52%
600	0.56%	37.54%	25.24%	24.90%	6.34%	0.86%	0.35%	4.21%						87.68%	11.76%	0.00%
700	1.09%	36.09%	23.46%	23.11%	7.64%	1.25%	1.08%	6.28%						82.66%	16.26%	0.00%
800	1.67%	34.50%	21.77%	21.42%	7.92%	1.73%	2.68%	8.31%						77.69%	20.64%	0.00%
900	2.20%	32.61%	20.06%	19.72%	7.41%	2.33%	5.53%	10.15%						72.38%	25.42%	0.00%
1000	2.62%	30.25%	18.21%	17.89%	6.46%	3.08%	9.87%	11.61%						66.35%	31.03%	0.00%
1100	2.91%	27.42%	16.20%	15.90%	5.36%	3.94%	15.70%	12.59%						59.51%	37.58%	0.00%
1200	3.06%	24.21%	14.07%	13.80%	4.27%	4.85%	22.71%	13.03%						52.08%	44.86%	0.00%
1300	3.10%	20.82%	11.94%	11.70%	3.31%	5.74%	30.42%	12.96%						44.46%	52.43%	0.00%
1400	3.06%	17.50%	9.91%	9.71%	2.51%	6.53%	38.27%	12.50%						37.12%	59.82%	0.00%
1500	2.95%	14.43%	8.09%	7.92%	1.89%	7.18%	45.77%	11.78%						30.44%	66.61%	0.00%
1600	2.81%	11.74%	6.52%	6.38%	1.41%	7.67%	52.55%	10.92%						24.64%	72.55%	0.00%
1700	2.66%	9.48%	5.22%	5.10%	1.06%	8.01%	58.47%	10.01%						19.80%	77.55%	0.00%
1800	2.49%	7.62%	4.17%	4.08%	0.80%	8.23%	63.49%	9.12%						15.87%	81.64%	0.00%
1900	2.33%	6.14%	3.34%	3.26%	0.61%	8.34%	67.69%	8.29%						12.74%	84.93%	0.00%
2000	2.17%	4.97%	2.69%	2.62%	0.47%	8.38%	71.17%	7.53%						10.28%	87.56%	0.00%
2100	2.02%	4.04%	2.18%	2.12%	0.37%	8.38%	74.05%	6.84%						8.34%	89.64%	0.00%
2200	1.88%	3.32%	1.78%	1.74%	0.29%	8.33%	76.44%	6.22%						6.83%	91.29%	0.00%
2300	1.75%	2.74%	1.47%	1.43%	0.24%	8.26%	78.44%	5.67%						5.64%	92.61%	0.00%
2400	1.63%	2.29%	1.22%	1.19%	0.19%	8.18%	80.12%	5.18%						4.70%	93.67%	0.00%
2500	1.51%	1.93%	1.03%	1.00%	0.16%	8.09%	81.53%	4.75%						3.95%	94.53%	0.00%

(d) 2-naphthyl + methylacetylene, 0.03 atm.

T, K	allene	p1	p2	p3	p4	p5	p6	p7	i1	i5	i7	i8	i17	i18	3-ring total	2-ring total	stabilization
300	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	96.67%		0.00%	3.33%	0.00%	0.00%	0.00%	0.00%	100.00%
400	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	94.04%		0.05%	5.89%	0.00%	0.00%	0.00%	0.02%	99.98%
500	0.00%	0.00%	0.00%	0.00%	0.23%	0.02%	0.00%	0.09%	90.93%		0.37%	8.36%	0.31%	0.68%	0.00%	0.35%	100.00%
600	0.00%	0.00%	0.00%	0.00%	2.17%	0.23%	0.00%	0.97%	84.98%		1.52%	9.83%			0.00%	3.38%	96.33%
700	0.00%	0.01%	0.00%	0.00%	10.17%	1.10%	0.00%	4.63%	69.86%		5.19%	9.02%			0.02%	15.90%	84.07%
800	0.01%	0.04%	0.02%	0.03%	25.78%	2.81%	0.01%	11.66%	44.62%	6.28%	8.73%				0.08%	40.25%	59.62%
900	0.05%	0.11%	0.07%	0.08%	42.11%	4.64%	0.03%	18.79%	21.32%	3.35%	9.41%				0.26%	65.57%	34.08%
1000	0.16%	0.24%	0.14%	0.15%	52.96%	5.90%	0.10%	23.32%	9.48%		7.51%				0.53%	82.29%	16.99%
1100	0.35%	0.35%	0.20%	0.22%	58.62%	6.61%	0.21%	25.45%	3.24%		4.74%				0.77%	90.89%	7.98%
1200	0.55%	0.39%	0.22%	0.25%	61.87%	7.06%	0.33%	26.59%			2.73%				0.86%	95.85%	2.73%
1300	0.70%	0.35%	0.19%	0.23%	62.81%	7.24%	0.39%	26.84%			1.25%				0.77%	97.28%	1.25%
1400	0.77%	0.27%	0.14%	0.18%	63.31%	7.35%	0.41%	27.03%			0.53%				0.60%	98.10%	0.53%
1500	0.78%	0.20%	0.10%	0.14%	63.52%	7.42%	0.38%	27.24%			0.22%				0.44%	98.57%	0.22%
1600	0.78%	0.16%	0.07%	0.12%	63.56%	7.47%	0.35%	27.49%							0.35%	98.87%	0.00%
1700	0.73%	0.10%	0.04%	0.09%	63.48%	7.50%	0.29%	27.76%							0.24%	99.03%	0.00%
1800	0.69%	0.07%	0.03%	0.07%	63.32%	7.52%	0.24%	28.06%							0.17%	99.14%	0.00%
1900	0.65%	0.05%	0.02%	0.06%	63.12%	7.53%	0.20%	28.38%							0.13%	99.22%	0.00%
2000	0.61%	0.04%	0.01%	0.05%	62.88%	7.53%	0.17%	28.72%							0.10%	99.29%	0.00%
2100	0.57%	0.03%	0.01%	0.04%	62.61%	7.53%	0.14%	29.07%							0.08%	99.34%	0.00%
2200	0.54%	0.03%	0.00%	0.04%	62.32%	7.53%	0.11%	29.43%							0.07%	99.39%	0.00%
2300	0.51%	0.02%	0.00%	0.03%	62.01%	7.52%	0.09%	29.80%							0.06%	99.43%	0.00%
2400	0.48%	0.02%	0.00%	0.03%	61.69%	7.50%	0.08%	30.20%							0.05%	99.46%	0.00%
2500	0.46%	0.02%	0.00%	0.03%	61.34%	7.48%	0.06%	30.61%							0.04%	99.50%	0.00%

(e) 2-naphthyl + methylacetylene, 1 atm.

T, K	allene	p1	p2	p3	p4	p5	p6	p7	i1	i5	i7	i8	i17	i18	3-ring total	2-ring total	stabilization
300	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	96.70%		0.00%	3.30%			0.00%	0.00%	100.00%
400	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	94.19%		0.00%	5.81%			0.00%	0.00%	100.00%
500	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	91.72%		0.01%	8.25%			0.00%	0.01%	99.99%
600	0.00%	0.00%	0.00%	0.00%	0.09%	0.01%	0.00%	0.04%	89.36%		0.06%	10.43%			0.00%	0.14%	99.85%
700	0.00%	0.00%	0.00%	0.00%	0.71%	0.08%	0.00%	0.35%	86.51%		0.28%	12.05%			0.00%	1.14%	98.85%
800	0.00%	0.00%	0.00%	0.00%	3.61%	0.40%	0.00%	1.76%	80.81%	12.48%	0.90%				0.00%	5.77%	94.20%
900	0.00%	0.00%	0.00%	0.00%	11.63%	1.29%	0.00%	5.45%	68.43%	11.16%	1.99%				0.00%	18.37%	81.58%
1000	0.01%	0.01%	0.00%	0.01%	24.98%	2.80%	0.00%	11.24%	49.47%	8.41%	3.00%				0.01%	39.02%	60.88%
1100	0.03%	0.02%	0.01%	0.01%	39.26%	4.43%	0.02%	17.16%	30.21%	5.35%	3.39%				0.04%	60.87%	38.95%
1200	0.09%	0.04%	0.02%	0.03%	50.27%	5.72%	0.05%	21.81%	18.61%		3.25%				0.08%	77.85%	21.86%
1300	0.20%	0.06%	0.03%	0.05%	62.52%	7.15%	0.10%	26.60%			3.18%				0.14%	96.37%	3.18%
1400	0.33%	0.08%	0.03%	0.06%	63.14%	7.29%	0.16%	26.84%			2.00%				0.17%	97.43%	2.00%
1500	0.45%	0.08%	0.03%	0.07%	63.46%	7.38%	0.20%	27.11%			1.20%				0.18%	98.15%	1.20%
1600	0.54%	0.07%	0.03%	0.07%	63.52%	7.44%	0.22%	27.40%			0.69%				0.17%	98.58%	0.69%
1700	0.59%	0.06%	0.02%	0.06%	63.46%	7.48%	0.22%	27.71%			0.38%				0.15%	98.87%	0.38%
1800	0.61%	0.06%	0.02%	0.06%	63.31%	7.51%	0.20%	28.03%			0.20%				0.14%	99.05%	0.20%
1900	0.65%	0.05%	0.02%	0.06%	63.12%	7.53%	0.20%	28.38%							0.13%	99.22%	0.00%
2000	0.61%	0.04%	0.01%	0.05%	62.88%	7.53%	0.17%	28.72%							0.10%	99.29%	0.00%
2100	0.57%	0.03%	0.01%	0.04%	62.61%	7.53%	0.14%	29.07%							0.08%	99.34%	0.00%
2200	0.54%	0.03%	0.00%	0.04%	62.32%	7.53%	0.11%	29.43%							0.07%	99.39%	0.00%
2300	0.51%	0.02%	0.00%	0.03%	62.01%	7.52%	0.09%	29.80%							0.06%	99.43%	0.00%
2400	0.48%	0.02%	0.00%	0.03%	61.69%	7.50%	0.08%	30.20%							0.05%	99.46%	0.00%
2500	0.46%	0.02%	0.00%	0.03%	61.34%	7.48%	0.06%	30.61%							0.04%	99.50%	0.00%

(f) 2-naphthyl + methylacetylene, zero-pressure limit.

T, K	allene	p1	p2	p3	p4	p5	p6	p7	i1	i5	i7	i8	i17	i18	3-ring total	2-ring total	stabilization
300	0.00%	23.64%	18.07%	17.17%	3.40%	0.34%	0.00%	1.15%			35.86%	0.02%			58.88%	4.90%	35.88%
400	0.01%	30.21%	22.05%	21.83%	10.15%	1.05%	0.01%	3.94%			10.72%				74.10%	15.15%	10.72%
500	0.04%	27.16%	19.17%	18.95%	21.34%	2.25%	0.04%	9.08%			1.99%				65.28%	32.69%	1.99%
600	0.11%	20.06%	13.71%	13.54%	33.69%	3.60%	0.10%	15.18%							47.31%	52.57%	0.00%
700	0.24%	13.15%	8.73%	8.62%	43.91%	4.77%	0.19%	20.38%							30.50%	69.26%	0.00%
800	0.41%	8.17%	5.27%	5.21%	51.13%	5.64%	0.31%	23.85%							18.66%	80.93%	0.00%
900	0.58%	4.94%	3.11%	3.08%	55.87%	6.24%	0.41%	25.76%							11.13%	88.29%	0.00%
1000	0.72%	2.96%	1.81%	1.81%	58.94%	6.66%	0.49%	26.61%							6.58%	92.70%	0.00%
1100	0.82%	1.76%	1.05%	1.07%	60.91%	6.94%	0.53%	26.90%							3.89%	95.29%	0.00%
1200	0.87%	1.05%	0.61%	0.64%	62.17%	7.14%	0.54%	26.98%							2.31%	96.82%	0.00%
1300	0.88%	0.63%	0.36%	0.39%	62.93%	7.28%	0.51%	27.02%							1.38%	97.74%	0.00%
1400	0.86%	0.39%	0.21%	0.25%	63.36%	7.37%	0.46%	27.11%							0.84%	98.30%	0.00%
1500	0.82%	0.24%	0.12%	0.17%	63.54%	7.43%	0.40%	27.27%							0.53%	98.65%	0.00%
1600	0.78%	0.16%	0.07%	0.12%	63.56%	7.47%	0.35%	27.49%							0.35%	98.87%	0.00%
1700	0.73%	0.10%	0.04%	0.09%	63.48%	7.50%	0.29%	27.76%							0.24%	99.03%	0.00%
1800	0.69%	0.07%	0.03%	0.07%	63.32%	7.52%	0.24%	28.06%							0.17%	99.14%	0.00%
1900	0.65%	0.05%	0.02%	0.06%	63.12%	7.53%	0.20%	28.38%							0.13%	99.22%	0.00%
2000	0.61%	0.04%	0.01%	0.05%	62.88%	7.53%	0.17%	28.72%							0.10%	99.29%	0.00%
2100	0.57%	0.03%	0.01%	0.04%	62.61%	7.53%	0.14%	29.07%							0.08%	99.34%	0.00%
2200	0.54%	0.03%	0.00%	0.04%	62.32%	7.53%	0.11%	29.43%							0.07%	99.39%	0.00%
2300	0.51%	0.02%	0.00%	0.03%	62.01%	7.52%	0.09%	29.80%							0.06%	99.43%	0.00%
2400	0.48%	0.02%	0.00%	0.03%	61.69%	7.50%	0.08%	30.20%							0.05%	99.46%	0.00%
2500	0.46%	0.02%	0.00%	0.03%	61.34%	7.48%	0.06%	30.61%							0.04%	99.50%	0.00%

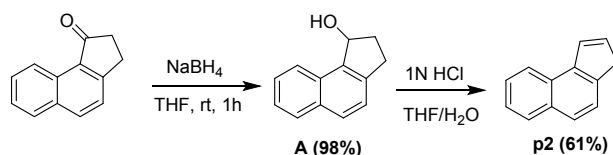
Synthesis of C₁₃H₁₀ isomers

General information

¹H (400 MHz) and ¹³C (100.6 MHz) NMR spectra were recorded at ambient temperature in solution of CDCl₃. Reaction progress was monitored by TLC on Merck Kieselgel 60-F254 sheets with product detection by 254 nm light. Products were purified by column chromatography using Merck Kieselgel 60 (230-400 mesh). Reagent grade chemicals were used and solvents were dried by reflux and distillation from CaH₂ under N₂ unless otherwise specified.

Synthesis of 3*H*-benz[e]indene **p2**

The 3*H*-benz[e]indene^{1,2} **p2** was synthesized by NaBH₄ reduction of commercially available 2,3-dihydro-1*H*-cyclopenta[a]naphthalene-1-one (**Scheme 1**) and β-elimination of the resulted secondary alcohol **A** with aqueous HCl.



Scheme 1. Synthesis of 3*H*-cyclopenta[a]naphthalene **p2**.

2,3-dihydro-1*H*-cyclopenta[a]naphthalene; **A**.

NaBH₄ (98 mg, 2.58 mmol) was added portion wise to a stirred solution of commercially available 2,3-dihydro-1*H*-cyclopenta[a]naphthalene-1-one (470 mg, 2.58 mmol) in dry MeOH/THF (2;1) at 0 °C (ice-bath). After 5 min, the reaction mixture was allowed to warm to ambient temperature and stirring was continued for 1 h. Water (1 mL) was then added to quench the reaction. The mixture was concentrated under reduced pressure and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated. The residue was column chromatographed (EtOAc in hexane 10-20%) to give 2,3-dihydro-1*H*-cyclopenta[a]naphthalene **A** (465 mg, 98%) as a white solid: ¹H NMR δ 1.80 (s, 1H), 2.15-2.23 (m, 1H), 2.56-2.65 (m, 1H), 2.95-3.02 (m, 1H), 3.26-3.34 (m, 1H), 5.79 (d, *J* = 4.8 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.44-7.48 (m, 1H), 7.52-7.56 (m, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H); ¹³C NMR δ 31.06, 35.48, 75.97, 123.52, 124.02, 125.29, 126.73, 128.66, 129.61, 130.32, 133.19, 139.29, 141.78.

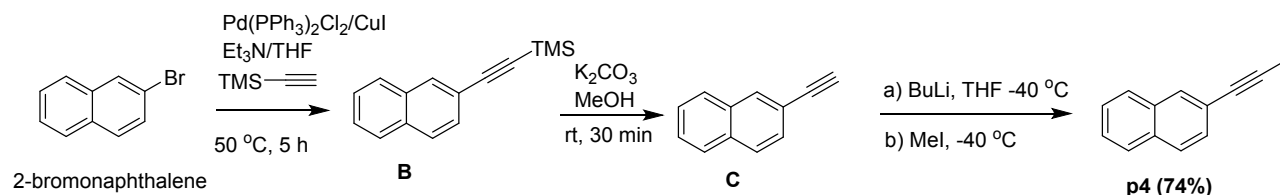
3*H*-benz[e]indene; **p2**.

The secondary alcohol **A** (440 mg, 2.39 mmol) was dissolved in THF/H₂O (20 mL, 1:1). Aqueous 1N HCl (6.0 mL, 6 mmol) was then added and the reaction mixture was refluxed at 105 °C for 6 h. After removing THF, the reaction mixture was transferred to a separatory funnel and extracted with EtOAc. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered,

and evaporated at reduced pressure. The residue was column chromatographed (*n*-hexane) to give 3*H*-benz[*a*]indene **p2** (240 mg, 61%) as a white solid: ^1H NMR δ 3.59 (s, 2H), 6.77 (d, J = 5.6 Hz, 1H), 7.46-7.56 (m, 3H), 7.66 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 8.15 (d, J = 8.4 Hz, 1H); ^{13}C NMR δ 40.51, 122.57, 123.95, 124.89, 125.02, 125.70, 127.99, 128.50, 129.70, 132.74, 134.40, 141.12, 141.38.

Synthesis of 2-(prop-1-yn-1-yl)naphthalene **p4**

The 2-(prop-1-yn-1-yl)naphthalene **p4** was synthesized by Sonogashira coupling between 2-bromonaphthalene and TMS-acetylene (**Scheme 2**) followed by desilylation. The resulted 2-ethynylnaphthalene **C** was converted to alkynide with BuLi and methylated with MeI yielding 2-(prop-1-yn-1-yl)naphthalene **p4**.³



Scheme 2. Synthesis of 2-(prop-1-yn-1-yl)naphthalene **p4**.

Trimethyl(naphthalen-2-ylethynyl)silane; **B**.

$\text{Pd(PPh}_3)_2\text{Cl}_2$ (35.1 mg, 0.05 mmol) and Cu(I)I (19.1 mg, 0.1 mmol) were added to anhydrous THF (10 mL) and anhydrous Et_3N (1.5 mL, 1090 mg, 10.7 mmol) placed in flame-dried round bottom flask equipped with a stir bar. Then 2-bromonaphthalene (1035 mg, 5.0 mmol) was added followed by TMS-acetylene (832 μL , 575 mg, 5.85 mmol). The resulting mixture was stirred at 50 $^\circ\text{C}$ for 5 h [progress of the reaction was monitored by TLC (hexane)]. The reaction mixture was then diluted with hexane and filtered through a short pad of silica. Volatiles were evaporated and the residue was column chromatographed (*n*-hexane) to give trimethyl(naphthalen-2-ylethynyl)silane **B** (500 mg, 45%) as a light yellow solid: ^1H NMR δ 0.29 (s, 9H), 7.46-7.52 (m, 3H), 7.75-7.78 (m, 3H), 8.00 (s, 1H); ^{13}C NMR δ 0.17, 94.69, 105.62, 120.61, 126.65, 126.87, 127.89, 127.94, 128.00, 128.74, 132.15, 133.05, 133.07.

2-Ethynylnaphthalene; **C**.

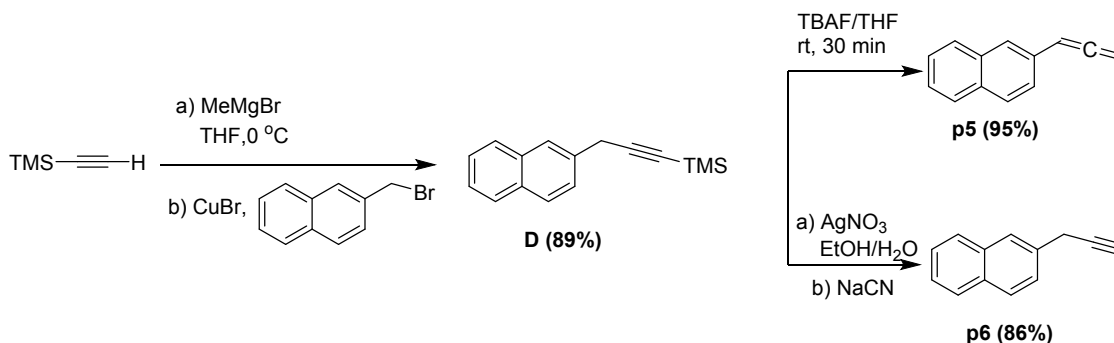
Anhydrous K_2CO_3 (300 mg, 2.2 mmol) was added to a stirred solution of **B** (480 mg, 2.14 mmol) in 10 mL MeOH at room temperature. After for 30 min, volatiles were evaporated and the residue was column chromatographed (*n*-hexane) to give **C** (300 mg, 92%) as a light yellow solid: ^1H NMR δ 3.15 (s, 1H), 7.49-7.55 (m, 3H), 7.78-7.84 (m, 3H), 8.04 (s, 1H); ^{13}C NMR δ 77.53, 84.17, 119.56, 126.76, 127.05, 127.92, 127.93, 128.17, 128.70, 132.46, 133.00, 133.21.

2-(Prop-1-yn-1-yl)naphthalene; **p4**.

A stirring solution of terminal alkyne **C** (204 mg, 1.34 mmol) in dry THF (10 mL) was cooled to -40 °C and *n*-BuLi (1.6 M/hexane, 1.70 mL, 2.72 mmol) was added. After 1 h, iodomethane (176 μ L, 400 mg, 2.82 mmol) was added dropwise at -40 °C and stirred for 1 h at room temperature. The mixture was poured into a saturated aqueous solution of NH₄Cl and extracted with Et₂O. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated at reduced pressure. The residue was column chromatographed (*n*-hexane) to give 2-(Prop-1-yn-1-yl)naphthalene **p4** (160 mg, 74%) as a gummy solid: ¹H NMR δ 2.12 (s, 2H), 7.45-7.51 (m, 3H), 7.76-7.82 (m, 3H), 7.93 (s, 1H); ¹³C NMR δ 4.54, 80.25, 86.34, 121.54, 126.38, 126.48, 127.72, 127.82, 127.96, 128.80, 131.14, 132.63, 133.22.

Synthesis of 2-(propa-1,2-dien-1-yl)naphthalene **p5** and 2-(prop-2-yn-1-yl)naphthalene **p6**

The 2-(propa-1,2-dien-1-yl)naphthalene **p5** and 2-(prop-2-yn-1-yl)naphthalene **p6** were synthesized from the commercially available 2-bromomethylnaphthalene by modifying reported protocols.^{4,5} Thus, treatment of trimethylsilylacetylene with MeMgBr generate alkynide which was reacted with 2-bromomethylnaphthalene (**Scheme 1**) in presence of CuBr to give **D**. Then treatment of **D** with TBAF in THF at rt gave expected product **p5**. On the other hand, treatment of **D** with AgNO₃/NaCN in EtOH/H₂O at rt gave expected isomeric product **p6**.



Scheme 3. Synthesis of 2-(propa-1,2-dien-1-yl)naphthalene **p5** and 2-(prop-2-yn-1-yl)naphthalene **p6**.

Trimethyl(3-(naphthalene-yl)prop-1-yn-yl)silane; **D**.

To a stirred solution of trimethylsilylacetylene (1.4 mL, 966.0 mg, 10.0 mmol) in dry THF (5 mL) was added dropwise MeMgBr (3 M/Et₂O, 3.4 mL, 10.0 mmol) at 0 °C under N₂. The stirring was continued for 30 min at 0 °C and another 30 min at room temperature. Then CuBr (212.2 mg, 1.5 mmol) was added and stirring was continued for 30 min. Next, 2-bromomethylnaphthalene was added and the resulting mixture was refluxed (80 °C, oil bath) for 5 h. After being cooled to room temperature, the mixture was poured into a saturated aqueous solution of NH₄Cl and extracted with Et₂O. The organic phase was separated, dried over

anhydrous Na₂SO₄, filtered, and evaporated at reduced pressure. The residue was column chromatographed (*n*-hexane) to give trimethyl(3-(naphthalene-yl)prop-1-yn-1-yl)silane **D** (530 mg, 89%) as a white solid: ¹H NMR δ 0.22 (s, 9H), 3.82 (s, 2H), 7.45-7.50 (m, 3H), 7.80-7.84 (m, 4H); ¹³C NMR δ 0.30, 26.54, 87.36, 104.38, 125.65, 125.75, 126.31, 126.41, 126.50, 126.63, 127.81, 132.47, 133.63, 133.98.

2-(Propa-1,2-dien-1-yl)naphthalene; p5.

The trimethylsilane product **D** (160 mg, 0.67 mmol) was dissolved in THF (5 mL) under N₂. A solution of tetra-*n*-butylammonium fluoride (TBAF) in THF (1 M/THF, 810 μL, 0.81 mmol) was added dropwise and stirring was continued for 30 min at room temperature. During this time, the reaction mixture turned to deep pink color. The mixture was poured into a saturated aqueous solution of NH₄Cl and extracted with Et₂O. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated at reduced pressure. The residue was column chromatographed (*n*-hexane) to give 2-(propa-1,2-dien-1-yl)naphthalene **p5** (106 mg, 95%) as a white solid: ¹H NMR δ 5.23 (d, *J* = 6.8 Hz, 2H), 6.35 (t, *J* = 6.8 Hz, 1H), 7.41-7.52 (m, 3H), 7.67 (s, 1H), 7.77-7.81 (m, 3H); ¹³C NMR δ 79.25, 94.45, 124.71, 124.83, 125.49, 125.60, 126.31, 127.84, 128.42, 131.55, 132.74, 133.82, 210.48.

2-(Prop-2-yn-1-yl)naphthalene; p6.

A stirred solution of trimethylsilane product **D** (190 mg, 0.80 mmol) in EtOH (4 mL) was treated with AgNO₃ (0.35 M, 3.5 mL, 1.23 mmol) in EtOH/H₂O (2.3:1). The resulting mixture was covered with aluminum foil and stirred for 2 h at room temperature (a white solid was precipitated during this time). An aqueous solution of NaCN (7.6 M, 1 mL, 7.6 mmol) was then added and stirring was continued until the disappearance of white precipitate. The reaction mixture extracted with Et₂O. The organic phase was separated, dried over anhydrous Na₂SO₄, filtered, and evaporated at reduced pressure. The residue was column chromatographed (*n*-hexane) to give 2-(prop-2-yn-1-yl)naphthalene **p6** (110 mg, 83%) as a white solid: ¹H NMR δ 2.26 (t, *J* = 2.4 Hz, 1H), 3.78 (d, *J* = 2.0 Hz, 2H), 7.44-7.50 (m, 3H), 7.81-7.84 (m, 4H); ¹³C NMR δ 25.51, 70.90, 82.03, 125.74, 126.28, 126.36, 126.51, 127.74, 127.81, 128.33, 128.42, 132.50, 133.65.

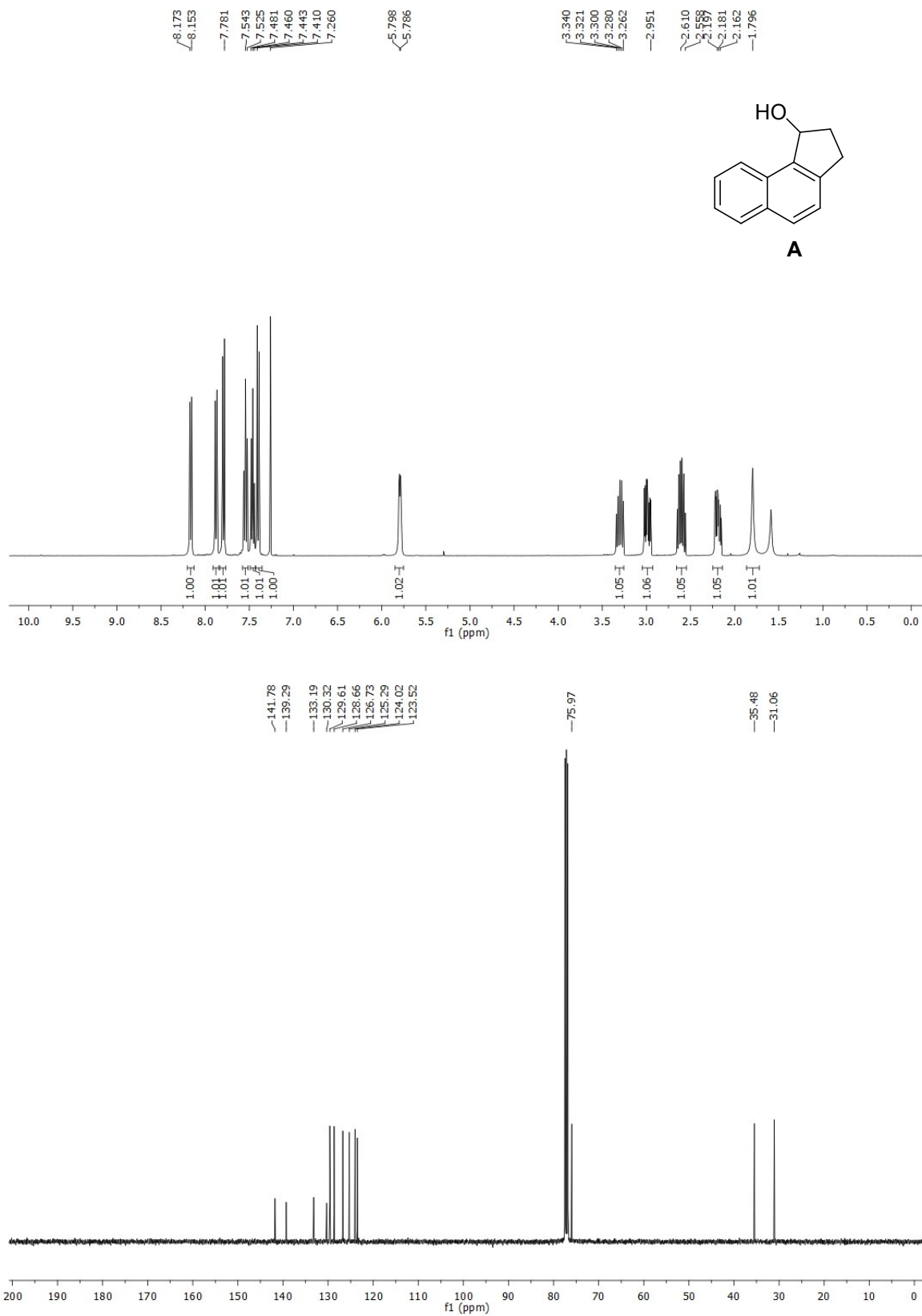


Figure S1. ^1H NMR and ^{13}C NMR spectra of compound **A** in CDCl_3 .

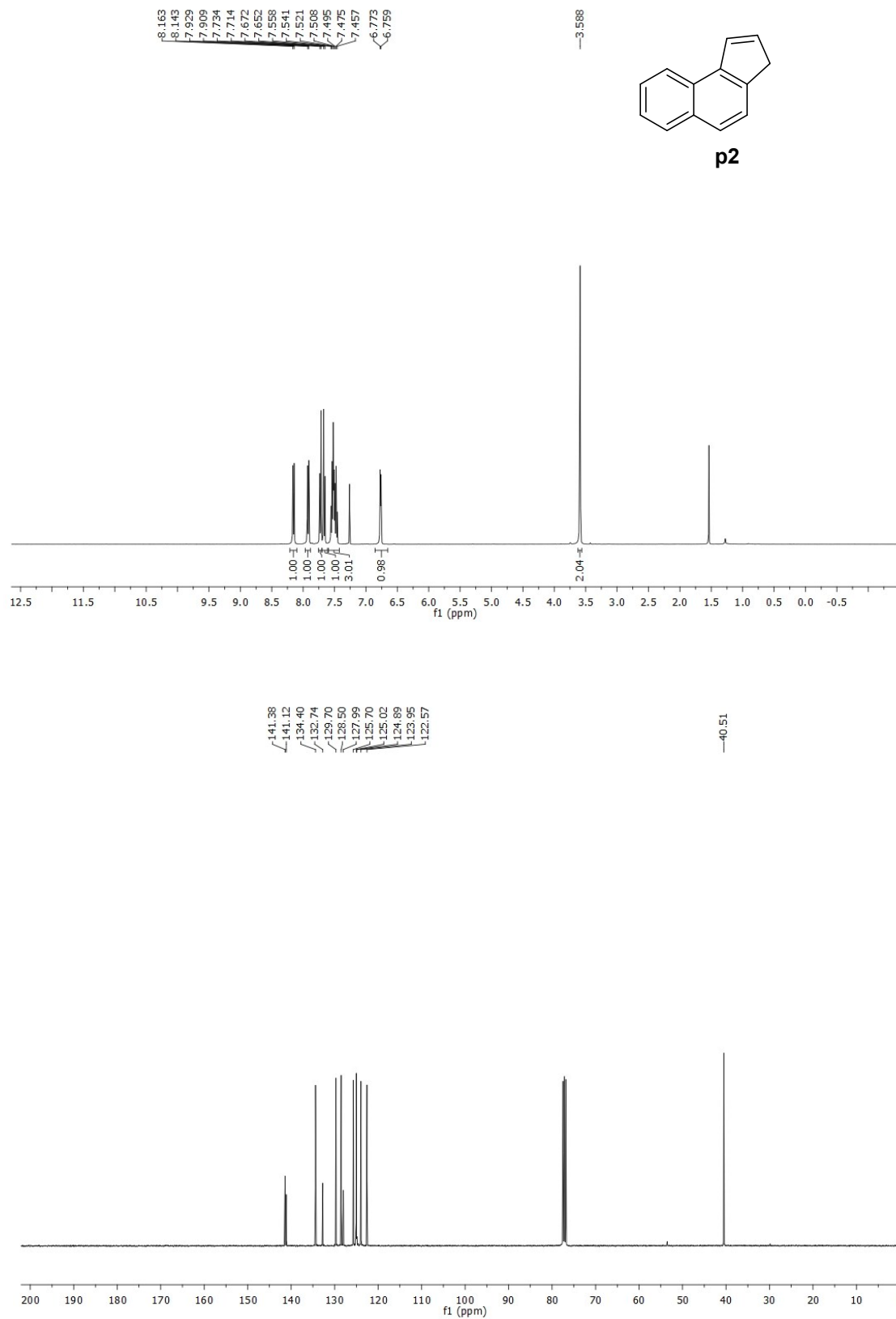


Figure S2. ¹H NMR and ¹³C NMR spectra of compound **p2** in CDCl₃.

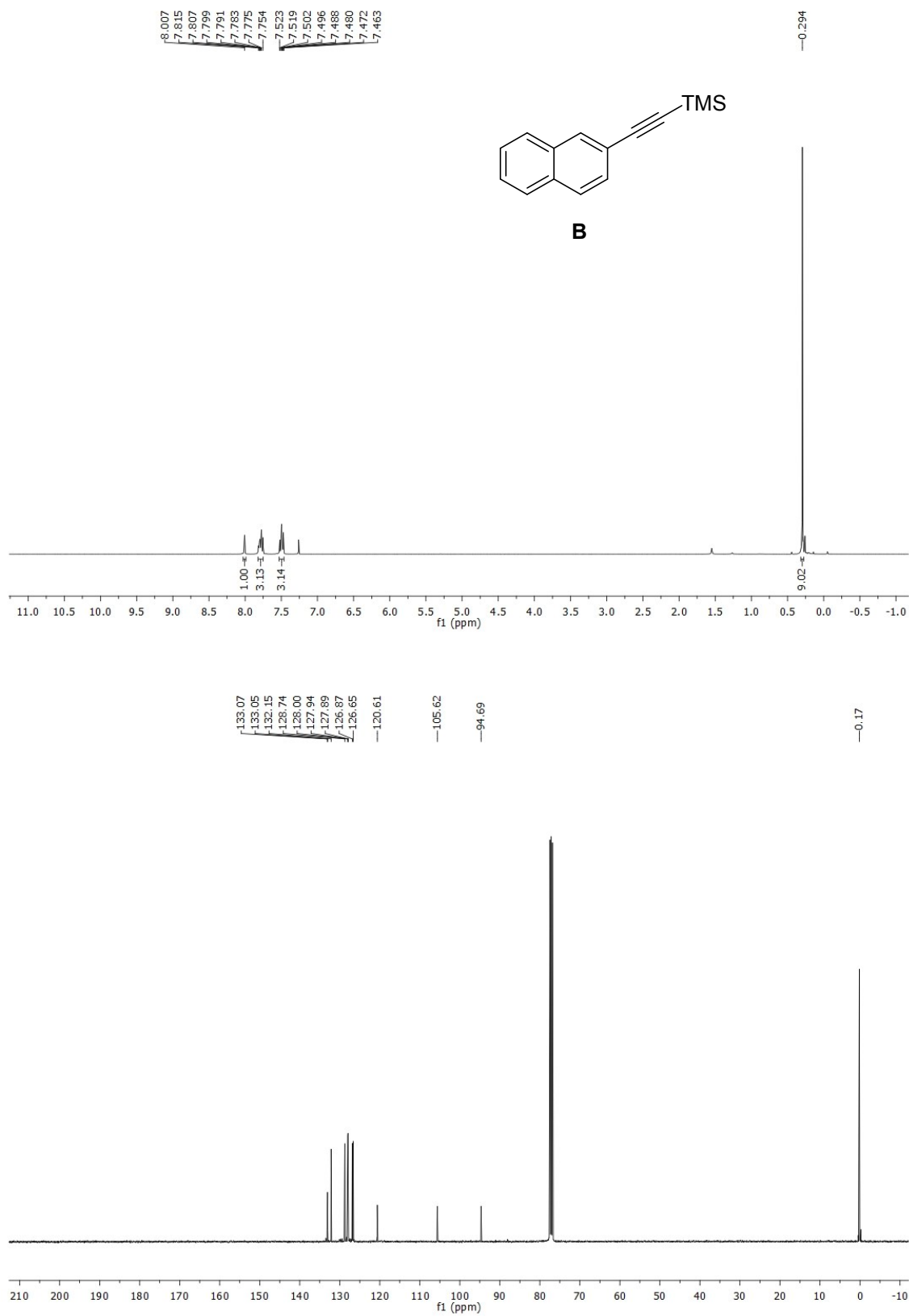


Figure S3. ¹H NMR and ¹³C NMR spectra of compound **B** in CDCl₃.

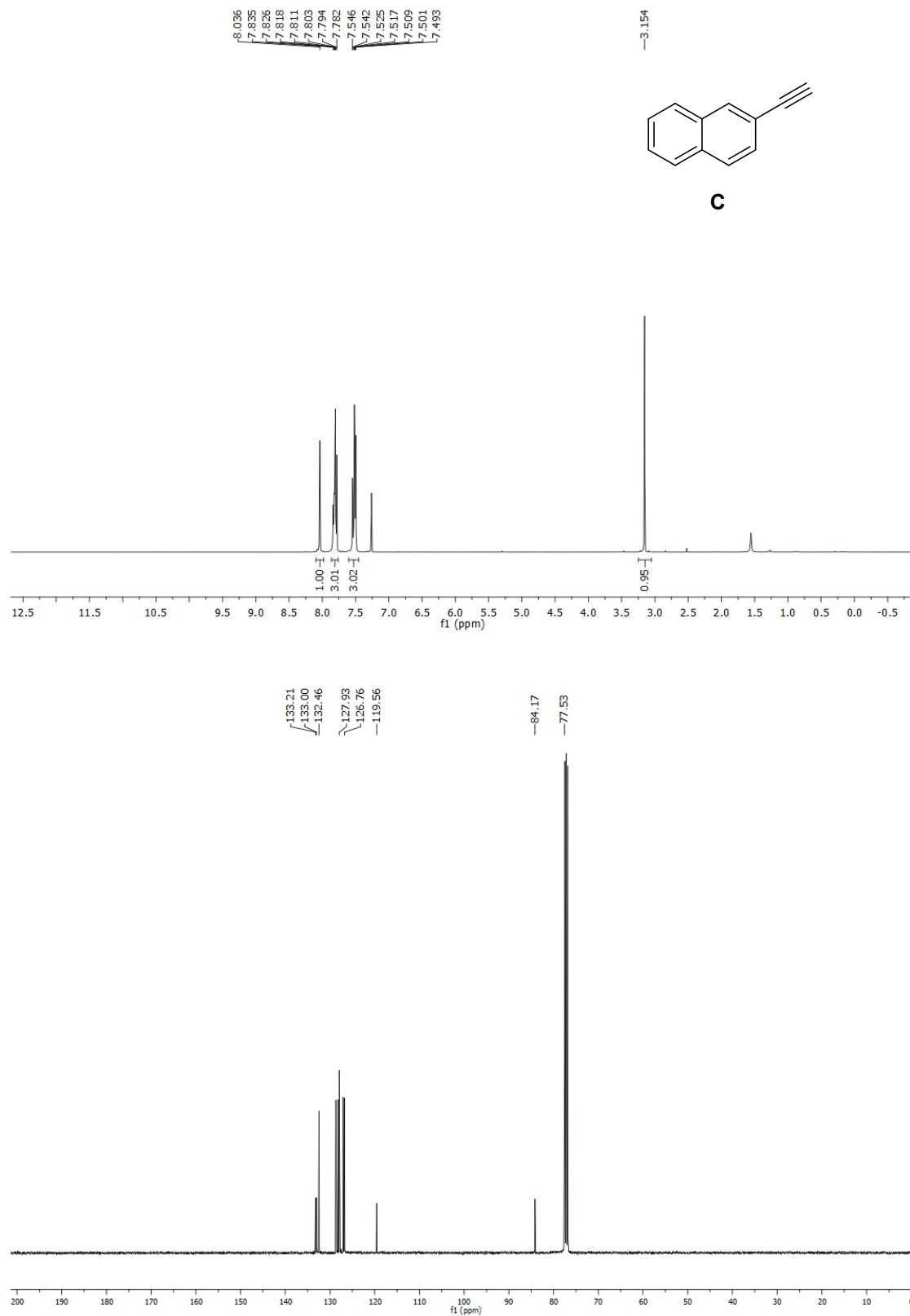


Figure S4. ^1H NMR and ^{13}C NMR spectra of compound **C** in CDCl_3 .

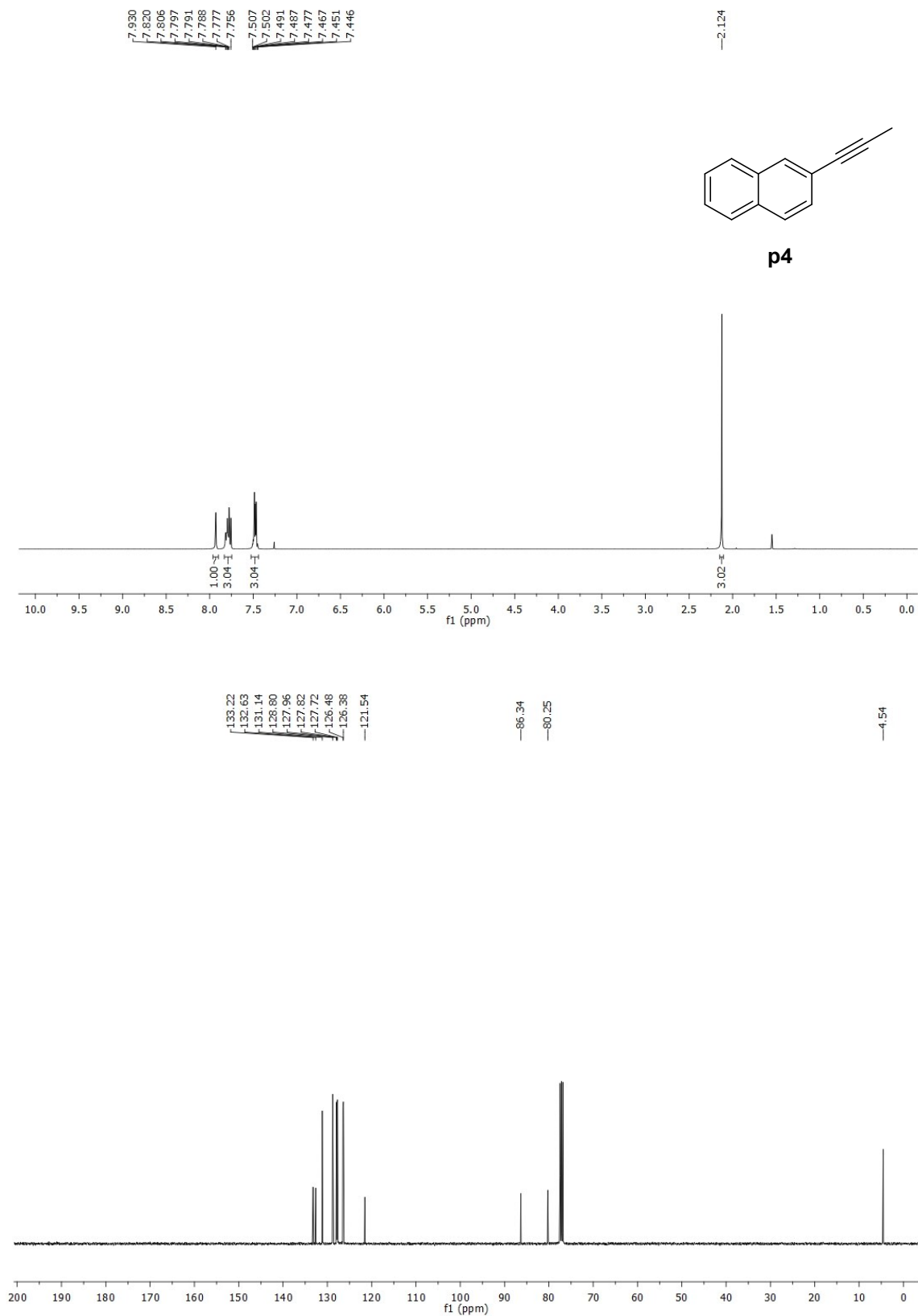


Figure S5. ¹H NMR and ¹³C NMR spectra of compound **p4** in CDCl₃.

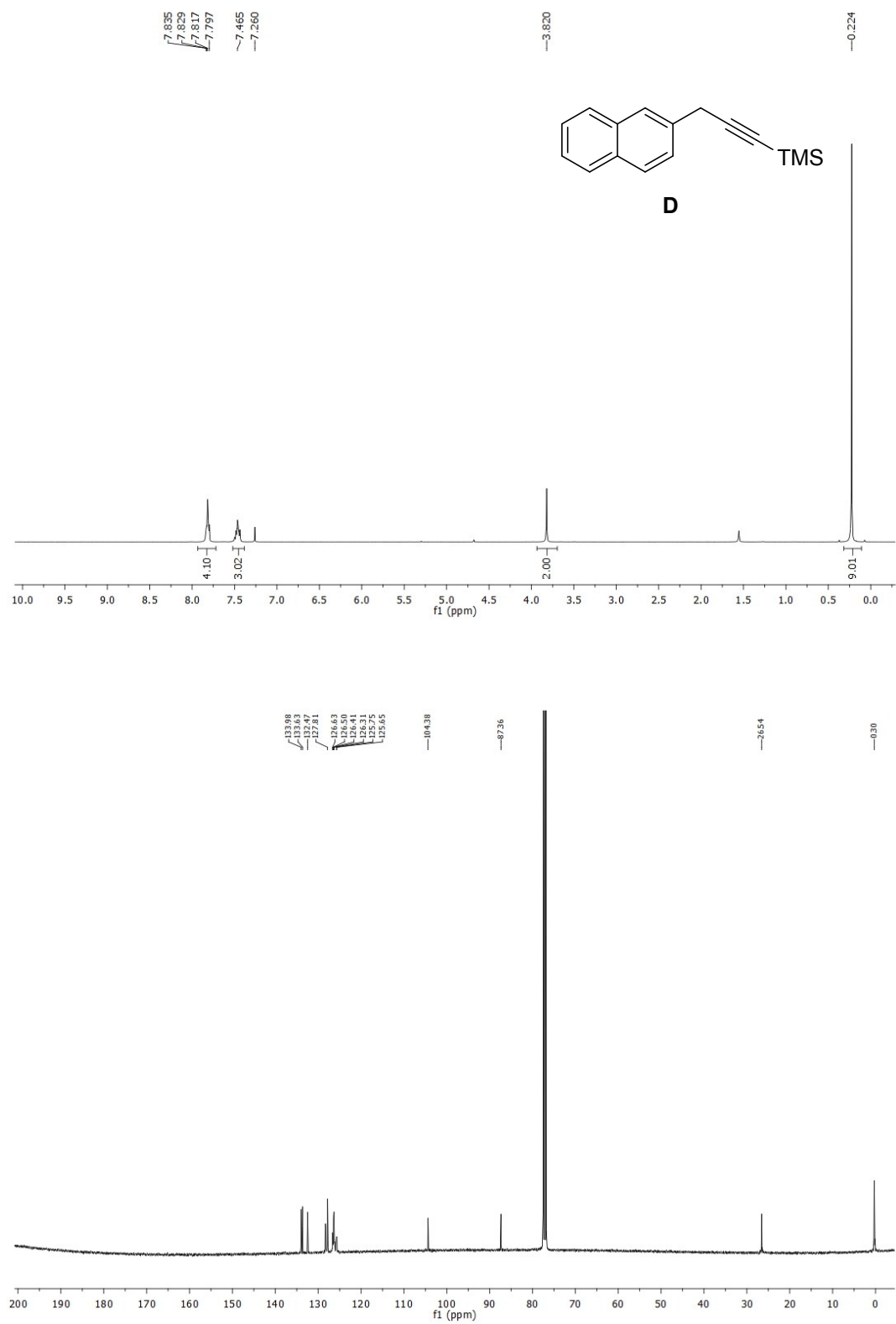


Figure S6. ^1H NMR and ^{13}C NMR spectra of compound **D** in CDCl_3 .

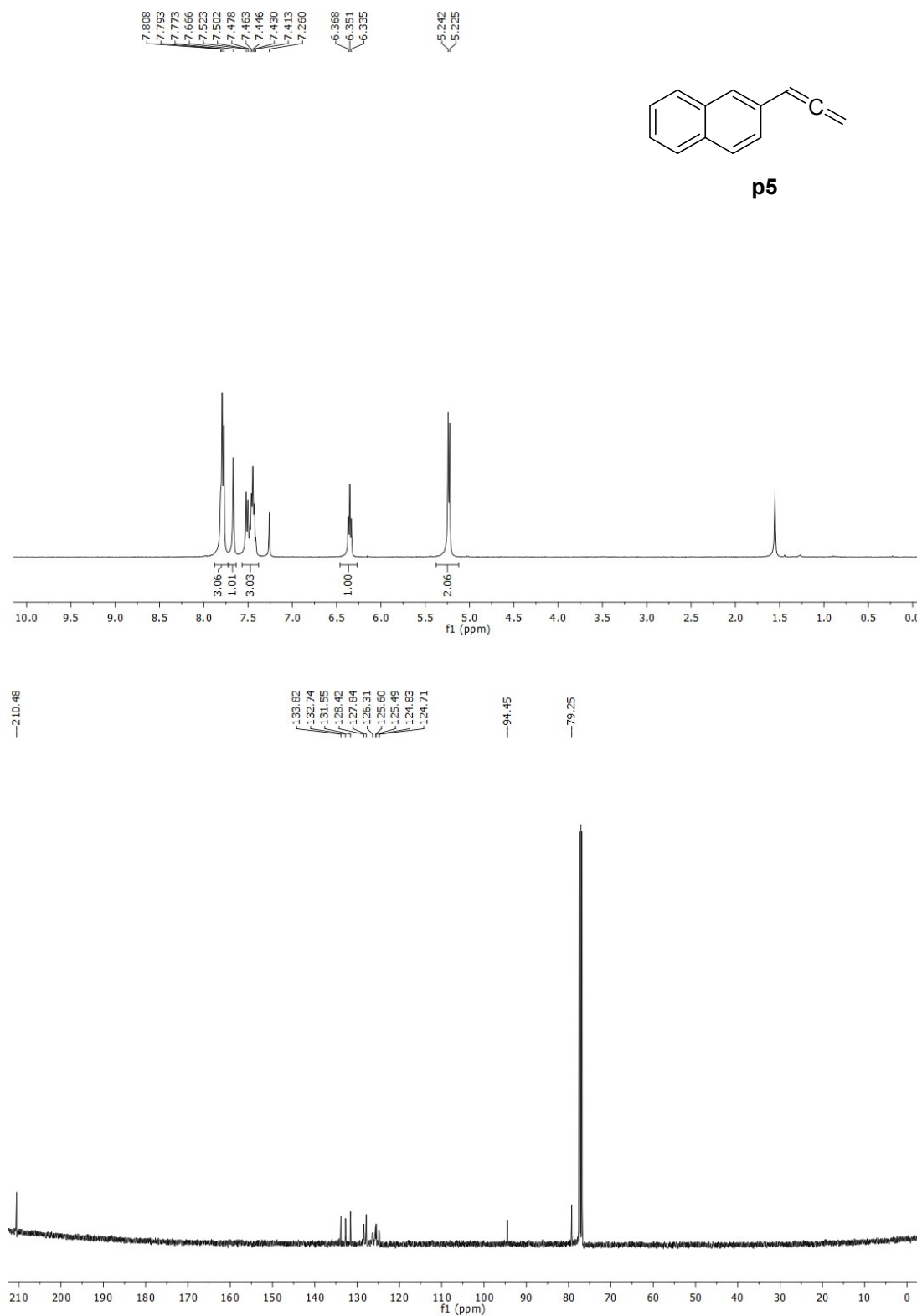


Figure S7. ¹H NMR and ¹³C NMR spectra of compound **p5** in CDCl₃.

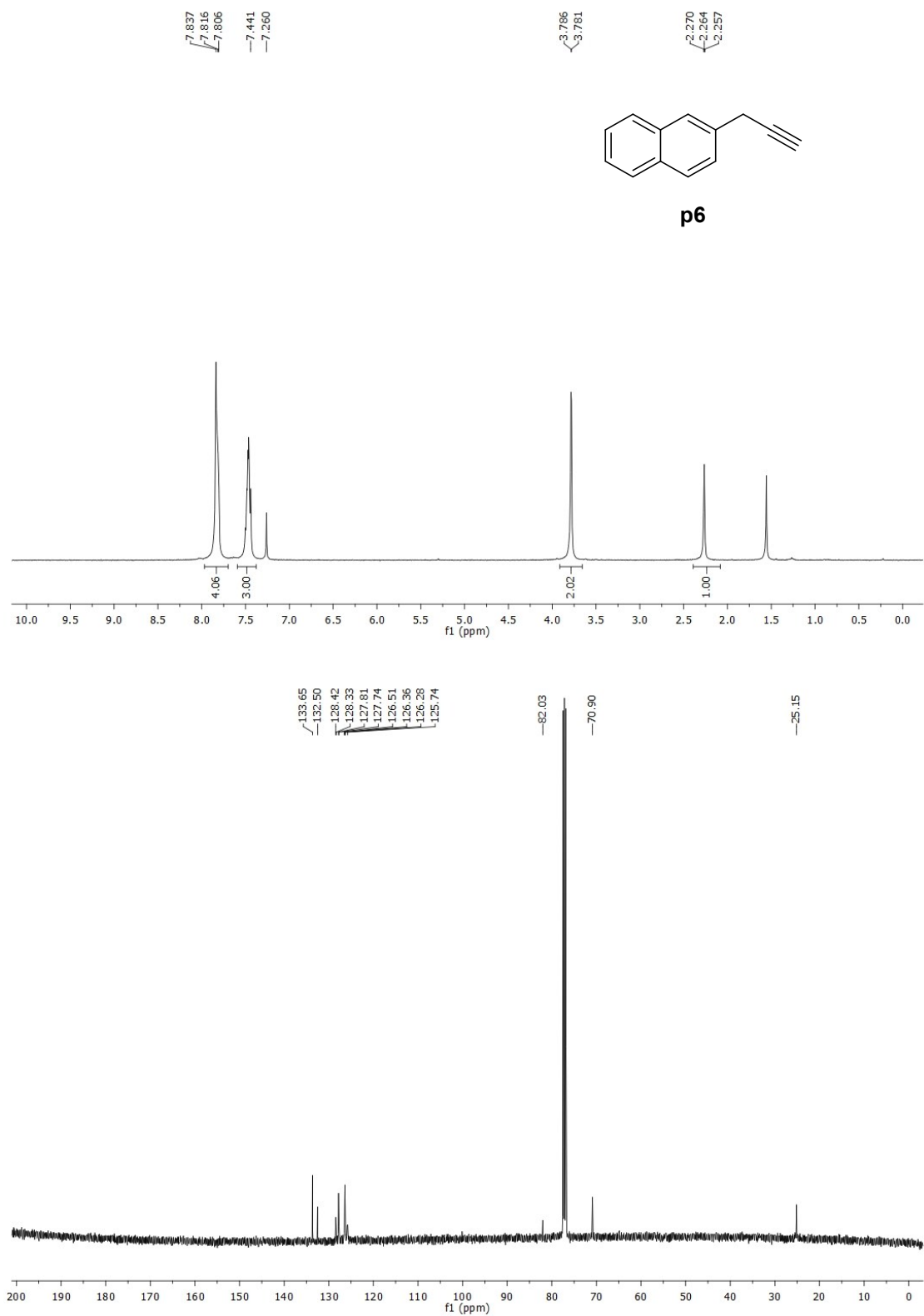


Figure S8. ¹H NMR and ¹³C NMR spectra of compound **p6** in CDCl₃.

Input file for RRKM-ME calculations using the MESS package

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Jasper calc 11/22/15
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Jasper calc 11/22/15
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C  1.2918507634 -0.124241909 -0.1453977948
C  -0.3068117665 1.7119122983 -0.119187446
C  0.9881657417 1.2681985549 -0.1770470289
C  -2.744431032 1.2297651957 0.0307665076
C  -2.1882754817 -1.5150817931 0.0696942526
C  -1.3941622674 0.8028666155 -0.0305623304
C  -1.1071299383 -0.5978960696 -0.0110504274
C  2.67925489 -0.6340720119 -0.1933110311
C  3.8077459159 0.0302758083 -0.0497169847
H  -4.7974610346 0.654533399 0.1570208867
H  0.452091923 -2.0878144684 -0.0566180181
H  -4.3024918708 -1.7808242354 0.1913675077
H  -0.5178429421 2.7761004466 -0.1492002026
H  1.7930855397 1.9863473004 -0.2676749216
H  -2.958035731 2.2936267212 0.0146461238
H  -1.9718822389 -2.5782951365 0.0844407903
H  2.7508480758 -1.7115002986 -0.3562439157
C  4.421803946 1.334564912 0.2222343687
H  3.7985584832 1.9494104854 0.8866524564
H  4.5914021351 1.8964819324 -0.7035418513
H  5.3952734188 1.2179286496 0.7107226747
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
28.0073 83.5010 109.1892
133.5065 186.7240 218.9466
259.5024 380.5428 387.0248
394.0610 410.8365 485.4407
524.2916 526.6618 601.8770
636.8480 648.3648 738.7510
752.3383 780.5739 781.7454
810.0416 835.0317 866.0476
877.0535 914.9444 940.3285
962.6356 974.2734 975.8261
995.1570 1013.2985 1030.9135
1041.9786 1146.1289 1173.7207
1181.0345 1189.9129 1237.2826
1279.0685 1284.8456 1294.2975
1385.9239 1394.0085 1399.3125
1405.9301 1456.8673 1470.0948
1473.6468 1499.1801 1542.9988
1606.3307 1639.2229 1665.1396
1736.2357 2977.4980 3038.6055
3054.4557 3070.7042 3154.4580
3157.0102 3160.0068 3162.9261
3174.6304 3187.4110 3196.9874
ZeroEnergy[kcal/mol] -40.05
ElectronicLevels[1/cm] 1
0 2
End
End
!-----

```

```

!-----well_i3-----
Well      i3
Species
RRHO
Geometry[angstrom]  24
C   -3.7793940786  0.6161594701  0.0318477038
C    0.0576709913 -1.1615330245 -0.1010372283
C   -3.6516766954 -0.7828643422  0.0758194527
C    1.2803251925 -0.3568229779 -0.184743143
C   -0.1645889384  1.6502669927 -0.2018095308
C    1.0666181449  1.1038378028 -0.2432883466
C   -2.6400236834  1.4099034167 -0.0575496682
C   -2.4057431346 -1.3740149902  0.0320677579
C   -1.3633241034  0.8433031365 -0.1033352434
C   -1.2210409763 -0.5885314532 -0.0566560185
H   -4.7610905525  1.0739688532  0.0663799734
H    0.1611075674 -2.2417241099 -0.0726527985
H   -4.5397865955 -1.4017679916  0.1444129595
H   -0.2822350844  2.7289620081 -0.2463466364
H    1.9484145839  1.7322293921 -0.3224725178
H   -2.7352761005  2.4907902008 -0.0937091463
H   -2.3121070729 -2.4546222013  0.0659210831
C    2.5475857392 -0.9621836024 -0.8215462765
C    2.5849932845 -0.8995191783  0.4619733053
C    3.2030618912 -1.136089944  1.7813843889
H    2.973097597 -1.2501644062 -1.7697788167
H    2.5587744903 -1.7747520673  2.3929914636
H    3.3278691764 -0.1928453573  2.3217862867
H    4.1802343573 -1.615662627  1.6815129961
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
53.6692           99.3419           136.2830
169.6039          188.5506           255.3686
273.0203          353.4577           387.1398
424.7420          453.1640           465.6777
506.0938          514.6512           544.0269
619.5734          648.0808           673.7482
713.0608          724.2616           753.1318
758.8917          783.7029           809.5167
863.3294          873.9743           915.3368
924.9123          936.9861           972.2732
974.3715          985.5712          1043.2889
1050.9864         1055.8924          1103.1618
1142.8850         1157.7741          1167.1657
1206.2495         1249.5984          1280.9256
1293.7802         1343.5520          1404.5401
1409.7077         1427.8375          1457.5673
1475.1088         1480.0472          1504.6639
1560.2095         1608.0117          1646.2465
1869.7904         3022.5336          3079.9639
3094.5328         3145.6523          3152.9567
3156.3551         3159.1904          3167.4024

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3171.8447          3187.0607          3239.0798
ZeroEnergy[kcal/mol] -17.76
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i4-----
Well      i4
Species
RRHO
Geometry[angstrom]  24
C   -3.870470236  0.5830193474 -0.025368228
C    0.0695888063 -0.9098790155  0.3964388525
C   -3.6580103489 -0.7002010763  0.5284728125
C    1.16220445 -0.1654181838 -0.0055306459
C   -0.3413237244  1.6259937322 -0.6939989349
C    0.9263983041  1.1308389594 -0.5527997258
C   -2.8019378876  1.3490798996 -0.4275934364
C   -2.3827115884 -1.1927205717  0.6697927982
C   -1.475490344  0.8683640424 -0.2965206873
C   -1.2584606125 -0.4275017085  0.2636258666
H   -4.8813052812  0.9603666761 -0.1313587087
H    0.2054951291 -1.8970599626  0.8214994218
H   -4.5081097895 -1.2954728034  0.8423421124
H   -0.4939119141  2.6176357217 -1.1076454675
H    1.7721771771  1.7406861987 -0.8463102923
H   -2.9621785674  2.3347312214 -0.8523205507
H   -2.219472657 -2.1777074151  1.0949668958
C    3.577606494 -0.1594639932 -0.5093234002
C    2.5523785016 -0.6957838146  0.1238644501
C    2.7802841463 -1.9119922424  1.0040082127
H    3.7975826289  0.6406300124 -1.1984165277
H    2.2716124227 -2.7920846708  0.5982994163
H    2.396422121 -1.7415739328  2.0143057615
H    3.84391677 -2.1392974205  1.0687740052
Core  RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
25.1565          87.2535          169.1652
181.2959          218.6508          241.1144
321.5525          348.9185          396.9149
444.4098          471.2418          485.7804
497.0971          527.7866          553.4063
631.9661          636.6692          677.4083
690.3952          760.3538          781.9014
784.3128          802.1004          830.0262
872.0110          887.8667          907.7711
961.3933          963.2628          976.4720
996.2120          1004.8849          1042.6245
1048.9676          1084.9699          1151.8553
1174.8429          1184.0666          1210.4781
1242.8092          1282.6947          1292.8570

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1372.2286          1394.9065          1403.0848
1408.9817          1466.2942          1484.3235
1489.5704          1500.0564          1540.2911
1606.7357          1640.4797          1647.5405
1667.2374          3024.2219          3077.0074
3122.7573          3156.6554          3159.6615
3162.3911          3174.7330          3183.1604
3187.3135          3188.1533          3249.1780
ZeroEnergy[kcal/mol] -37.32
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i5-----
Well      i5
Species
RRHO
Geometry[angstrom]      24
C   -3.9077387148  0.6773913178 -0.0905455934
C   -0.1157330663 -1.194551157 -0.15462891
C   -3.8034629132 -0.6967954535 -0.4163876059
C   1.0377973322 -0.4864489743  0.1364697832
C   -0.3120751464  1.5115850361  0.4907242459
C   0.9130447211  0.891646305  0.4680288666
C   -2.7823314  1.4067393009  0.2050695535
C   -2.577428896 -1.3131178029 -0.4400617135
C   -1.4993468667  0.8006455902  0.1888744338
C   -1.3915031252 -0.5878995434 -0.1410284182
H   -4.8828470415  1.1511871366 -0.075436649
H   -0.0417423059 -2.2501089002 -0.3948466904
H   -4.7001208543 -1.2608675678 -0.6474669053
H   -0.3817680912  2.564657098  0.7433214518
H   1.7973240013  1.4700324271  0.703699412
H   -2.8601575431  2.4597880474  0.4554536116
H   -2.4961434741 -2.3659900317 -0.6891995248
C   2.5515754297 -2.3432553558 -0.4287218497
C   2.3709778599 -1.1499521889  0.1042913409
C   3.5632110714 -0.4165653754  0.7070209975
H   3.3741168957 -3.0263141644 -0.5798586853
H   3.3629655842 -0.1376119685  1.7460374489
H   3.7816576607  0.4993770289  0.1493477984
H   4.4554928825 -1.0426408039  0.6854476014
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
21.3639          87.3776          168.0427
181.6143          221.0295          239.9350
310.6918          348.8985          394.6243
450.8998          463.7035          483.6950
504.5956          528.9001          564.0251
627.5050          641.2032          671.5498
672.7411          760.1144          780.5829

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782.1215	829.1879	856.8731
865.1149	873.4814	921.3393
957.8148	963.2429	974.2890
996.1019	1009.3399	1030.2812
1039.7822	1079.2824	1155.2555
1173.6721	1185.6305	1211.0896
1245.7709	1282.0305	1290.6028
1377.1647	1391.1528	1401.1921
1405.2552	1465.6271	1484.3200
1486.3646	1500.7994	1543.2323
1602.9012	1633.5919	1649.5806
1672.5192	3022.0316	3077.6746
3115.4392	3156.5546	3161.0087
3161.9346	3164.8390	3174.8103
3187.2700	3194.0418	3237.5227

ZeroEnergy[kcal/mol] -37.12

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i6-----

Well i6

Species

RRHO

Geometry[angstrom] 24

C	-3.6711917155	0.3237348412	0.0146535213
C	0.3296297363	-0.9485507976	0.1032394351
C	-3.3952110283	-1.0608305392	0.1264846896
C	1.4219704157	-0.129863259	0.0323605833
C	-0.1960377272	1.7080570688	-0.1113440887
C	1.1035865176	1.2633462841	-0.0800062813
C	-2.6465483238	1.2352910613	-0.0635352145
C	-2.1002497998	-1.5139020216	0.1585240916
C	-1.2930693069	0.8126609823	-0.0342014643
C	-1.0169243803	-0.5965173273	0.0796364433
H	-4.7008483573	0.6621874026	-0.0090435915
H	-4.216881031	-1.7654168848	0.187031929
H	-0.3977823681	2.770490626	-0.1971908771
H	1.9097486765	1.9846192245	-0.14185622
H	-2.8601471504	2.2958832771	-0.1491889444
H	-1.8819927987	-2.5718136573	0.2439435489
H	2.3005106025	-2.6713794329	0.23600189
C	3.091013656	-1.9324714097	0.1728804469
C	2.8215874396	-0.6251688465	0.0674441829
C	3.9367162663	0.3884073265	-0.0192815744
H	4.1117004246	-2.2954507404	0.198610594
H	3.8859807829	0.9632921655	-0.9499212054
H	4.9075371785	-0.1070822644	0.0174539555
H	3.8925342907	1.1063609206	0.8063971499

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 66

16.8782	84.0209	160.4246
179.5530	228.7675	240.6793
316.6528	336.5418	402.5950
450.2503	477.6864	501.5406
507.1230	522.5373	546.5240
626.3906	632.9779	680.9454
725.1192	760.9675	772.6681
780.9788	826.0563	867.7764
874.5786	923.9828	932.6932
955.7678	963.1212	969.2093
996.8588	1026.3847	1037.0278
1068.4136	1135.7535	1155.6998
1175.4046	1186.8487	1238.6802
1266.1911	1286.1081	1353.5943
1366.7527	1387.5668	1411.1263
1435.6492	1450.3254	1485.3823
1491.3467	1500.5098	1520.6085
1577.2365	1631.7715	1654.6484
1688.9047	3018.7091	3064.9541
3110.8572	3137.2342	3157.1235
3163.7139	3168.7362	3181.0877
3186.4817	3191.4341	3221.4757

ZeroEnergy[kcal/mol] -36.45

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i7-----

Well i7

Species

RRHO

Geometry[angstrom] 24

C	3.6155696094	-0.1105140056	0.0190093877
C	-0.5014845523	0.8638744548	-0.1264613836
C	3.2148322678	1.2317834313	-0.1795161485
C	-1.4656384707	-0.1139073783	0.0113272358
C	0.2836470276	-1.788071777	0.2597047661
C	-1.0470144889	-1.4595786063	0.2062011377
C	2.6738239428	-1.1001716871	0.1639867863
C	1.8814776885	1.5578362258	-0.2281132392
C	1.2887240308	-0.7969376672	0.1176230604
C	0.8823957851	0.5597003729	-0.07970408
H	4.6713830311	-0.3542730487	0.0556010842
H	3.9676634304	2.0037194015	-0.2932799642
H	0.5836003498	-2.8185776427	0.4200256721
H	-1.7989636965	-2.229588406	0.3350151459
H	2.9787842648	-2.1304401022	0.3159337914
H	1.5733454042	2.5869980599	-0.3808280808
C	-3.7792884114	-0.595818933	-0.7752427608
C	-2.9212703888	0.2218569167	-0.0477851862
C	-3.3919115557	1.344493205	0.6242130182
H	-3.4160525017	-1.4474464032	-1.335204311
H	-4.8403819072	-0.3814458461	-0.8194363277

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H   -4.437843164 1.622019224 0.5694096001
H   -2.7404478041 1.9546097758 1.2356517491
H   -0.799667891 1.8927784359 -0.298334953
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
61.5257 83.7845 162.6394
185.2409 221.9911 315.7415
357.6780 392.8183 435.6403
486.3373 493.4387 525.2572
537.1731 545.4619 554.8259
598.2343 632.8777 679.8387
685.1655 761.2647 770.9907
781.7611 785.9993 803.3766
835.9515 875.6318 885.3958
920.2442 964.6880 964.7314
979.9108 982.8435 995.9836
1035.5727 1041.5489 1121.4455
1160.4613 1172.2825 1180.4777
1223.9415 1267.2190 1288.6271
1289.4845 1373.9898 1386.1491
1398.8525 1409.3421 1463.9660
1484.7258 1501.1796 1524.7840
1542.3290 1607.2459 1642.8188
1669.6550 3141.4305 3148.5334
3156.9577 3160.0793 3162.4895
3167.2797 3174.8597 3181.7476
3187.2782 3240.7412 3242.6521
ZeroEnergy[kcal/mol] -60.6
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i8-----
Well i8
Species
RRHO
Geometry[angstrom] 24
C -3.6069916063 0.0933806358 -0.014399582
C 0.5232274086 -0.8404488152 0.0338217063
C -3.1899025062 -1.2568891675 -0.0068253034
C 1.4784895278 0.1570933746 0.0423482363
C -0.2929262425 1.8300884249 0.0189298477
C 1.0371361099 1.5144865183 0.0344967368
C -2.6760639873 1.1057333976 -0.0061665353
C -1.8512260393 -1.5692468126 0.0088292287
C -1.2895990978 0.8158598092 0.00996429
C -0.8659863833 -0.5481749345 0.017649851
C 3.8491366344 0.8012376427 0.0674349468
C 2.9316624237 -0.1482223866 0.0592883826
C 3.3718327764 -1.6063109785 0.0674458013
H -4.6655371871 0.3274870649 -0.0267436435

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H    0.8171564505 -1.8833483741 0.0393652129
H   -3.9322153279 -2.0471411743 -0.0134284284
H   -0.6054076669 2.8693977329 0.0131960327
H    1.7844344467 2.299791198 0.0411659233
H   -2.9939069739 2.1433117662 -0.0119527367
H   -1.5305682111 -2.6060499414 0.0146519437
H    4.9274036997 0.8586785425 0.0792815085
H    3.0019323615 -2.1281980513 -0.8204528702
H    2.9819598016 -2.1243441365 0.9490296296
H    4.4590835886 -1.6846233349 0.0798918213
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
43.0655      88.5825      166.7133
182.4922     229.0412     242.0227
319.7288     349.1879     396.9751
454.5990     456.4615     486.2481
496.6197     526.9496     566.6385
630.1026     644.7449     673.3770
674.9245     761.2891     782.8811
783.7264     835.7384     859.1722
873.6733     882.1750     906.9230
957.3329     963.6825     985.1207
987.8938     995.7416    1031.7494
1043.1632    1084.3517    1151.8602
1174.4745    1178.8677    1215.9186
1247.1430    1288.6722    1294.3394
1373.8350    1393.7401    1399.5345
1412.8511    1467.2449    1486.3453
1487.3755    1500.7769    1539.7891
1608.0798    1639.9450    1649.1674
1667.8393    3022.9812    3078.6409
3116.4845    3155.6792    3157.9078
3161.2399    3174.0728    3179.3240
3180.8739    3187.4966    3237.4109
ZeroEnergy[kcal/mol] -38.25
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i9-----
Well      i9
Species
RRHO
Geometry[angstrom] 24
C   -3.6224535805 0.5374817594 0.0100480652
C    0.2266136829 -1.2130305838 0.0096705889
C   -3.4895000006 -0.8691735627 0.0050148338
C    1.3852976328 -0.4288133917 0.0144288793
C   -0.0224199211 1.5670425176 0.0196320969
C    1.2180035992 0.9979902801 0.0194897513
C   -2.5020873053 1.3394486925 0.0148269549

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C   -2.2432904943 -1.4493120826 0.0048408971
C   -1.2070171246 0.7743088153 0.0147812142
C   -1.0681050083 -0.6505541978 0.0096940827
C   2.6669993235 -1.0646723852 0.0141545649
C   5.1178511815 -1.1130041012 0.0172824154
C   3.9287779547 -0.4413560672 0.0182280034
H   -4.6105737925 0.983382751 0.0101300005
H   0.3223056565 -2.2945379609 0.0058070231
H   -4.3777207126 -1.4909526893 0.0012890767
H   -0.1224811306 2.6477651041 0.0235061236
H   2.092112531 1.6371475835 0.023283836
H   -2.6022398457 2.4200179961 0.0187008956
H   -2.1409804526 -2.5295201029 0.000986898
H   2.6599877602 -2.1520791973 0.010010755
H   6.0641821341 -0.5874439922 0.0201508282
H   5.1524837976 -2.1973141562 0.0137964275
H   3.9668111146 0.6446549716 0.0219097878
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
59.6049          129.6801          133.0886
166.1036          184.7885          309.7656
311.0694          327.2713          402.5542
433.6023          478.3128          524.7586
528.0305          582.4115          602.1255
639.2645          649.7429          755.4975
766.2610          775.0454          778.9246
815.1026          822.4663          849.9191
870.4852          892.0951          896.6836
955.8556          958.9410          973.9116
992.8064          999.8935          1003.2637
1042.5727         1142.5128          1170.8248
1174.9943         1198.7471          1213.2405
1238.6962         1274.4540          1290.5746
1308.6539         1334.1260          1388.0987
1392.5295         1416.2159          1461.5694
1489.7663         1500.2629          1537.2217
1542.1253         1590.1533          1629.9968
1650.4433         3132.5741          3138.5891
3146.7678         3156.2313          3157.9789
3160.1835         3163.3071          3175.3986
3188.2571         3191.9895          3230.7649
ZeroEnergy[kcal/mol] -65.69
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----well_i10-----
Well      i10
Species
RRHO
Geometry[angstrom] 24

```

```

C   -3.6493242995  0.5735470844 -0.1452412478
C   0.1809207835 -1.2019959828  0.079553051
C   -3.5216361778 -0.8333728293 -0.1985002434
C   1.3406804466 -0.4282139952  0.1853955444
C   -0.0596668419  1.5731744203  0.204270295
C   1.1774496942  0.9952579726  0.2662459192
C   -2.5311445483  1.3667699793 -0.0187907227
C   -2.2820470186 -1.4216085918 -0.1246777867
C   -1.240711587  0.7928549858  0.0572170653
C   -1.1076678019 -0.6312806704  0.0035604134
C   2.6121716974 -1.0955864181  0.2487196049
C   4.3509703305  0.6066362315 -0.407460719
C   3.9236128874 -0.5959007033  0.0829132066
H   -4.6330422153  1.0253001321 -0.2040189147
H   0.2712340122 -2.2832308288  0.038002107
H   -4.4092827237 -1.448001286 -0.297792788
H   -0.1566908321  2.6513600344  0.2826448993
H   2.046088422  1.6185423064  0.4251708504
H   -2.6275207971  2.446790116  0.0242682724
H   -2.1835360815 -2.5014318466 -0.1652823162
H   2.5490085545 -2.16270503  0.4431777195
H   5.4106395434  0.8196466966 -0.4758513948
H   3.6783615348  1.3606686303 -0.7923895868
H   4.7049340184 -1.3060974076  0.3476217717
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
49.8806           100.8988           136.5411
188.5402          216.3213           264.2685
333.3133          392.2019           406.7560
419.3030          479.6661           522.8956
528.0985          569.3201           623.4643
639.6441          656.2147           752.6535
760.1797          775.7416           780.5665
792.5792          831.4076           850.2815
871.3939          884.9528           901.7047
958.4768          962.3715           987.0937
992.5674          994.8571          1034.3766
1042.5503         1107.3842          1153.4326
1174.0998         1177.6220          1206.8484
1245.8912         1279.9150          1288.1722
1297.5482         1355.8983          1392.0175
1406.4136         1442.6882          1454.2988
1483.1624         1488.8671          1536.5418
1559.9195         1589.8976          1628.1535
1651.8929         3118.0955          3145.5017
3153.8292         3156.2958          3158.2009
3160.3063         3163.6236          3175.4937
3188.3735         3212.2464          3242.8691
ZeroEnergy[kcal/mol] -62.0
ElectronicLevels[1/cm]  1
0  2
End

```

```

End
!-----
!-----well_i11-----
Well      i11
Species
RRHO
Geometry[angstrom]  24
C   3.6489124218 0.5462303942 0.279666327
C  -0.2253820534 -1.176294578 -0.1967710789
C   3.4984420562 -0.8516308353 0.2346061825
C  -1.3049162502 -0.3892283221 -0.3943679749
C   0.1336824125 1.660064152 -0.2709344993
C  -1.1751775015 1.0908781965 -0.6952668057
C   2.5523386477 1.367443927 0.1279441993
C   2.2379882254 -1.4073677017 0.0499155108
C   1.248794483 0.8328980068 -0.0894673394
C   1.1014324422 -0.6058878223 -0.1112722853
C  -2.7232426078 -0.6687318257 -0.260697086
C  -2.509260277 1.6901266267 -0.1676270008
C  -3.4162953648 0.4793982327 -0.1447262979
H   4.6315956843 0.9781046525 0.4335349508
H  -0.3396752158 -2.2410764643 -0.0149442174
H   4.3630023996 -1.4944450668 0.3534179008
H   0.25849285 2.7381414412 -0.2402238959
H  -1.2353859948 1.1786115823 -1.7996515015
H   2.6695280764 2.445853943 0.1586251751
H   2.1213466026 -2.4865459009 0.037506886
H  -3.1426619725 -1.6657253035 -0.2003013665
H  -2.8873300539 2.5051902111 -0.7909769832
H  -2.3846357953 2.0912038271 0.8475475889
H  -4.4857942147 0.5480956275 0.0138176116
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
88.7557          111.4088          221.6221
249.3454         263.2087          371.1532
382.9945         404.5914          442.4998
468.1022         544.6548          560.5294
617.5827         660.3913          680.3771
705.0729         734.4981          744.4632
758.0152         776.1114          793.5343
827.0968         857.7670          891.5433
906.8091         945.0236          948.5227
967.9861         974.8884          984.4600
1023.8964        1042.6206         1098.6760
1120.7635        1138.6980         1147.9340
1162.2393        1175.6791         1202.9893
1244.4230        1252.2983         1281.8236
1284.9774        1318.5806         1339.8018
1367.1966        1382.6140         1403.8226
1451.3332        1483.0098         1499.8606
1555.3529        1599.9997         1616.1923
1661.5229        2851.0055         2997.4510

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3062.1087          3150.0163          3154.0831
3155.9141          3159.7789          3173.4004
3180.2784          3187.8540          3202.0502
ZeroEnergy[kcal/mol] -56.18
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i12-----
Well      i12
Species
RRHO
Geometry[angstrom]  24
C   3.7958464732  0.002016814  0.1551284761
C   -0.335209756 -0.8435048613 -0.1687935044
C   3.3546229925 -1.335141674  0.0640714803
C   -1.2945851304  0.2020163812 -0.1896048346
C   0.5227503231  1.8262721716  0.0121930197
C   -0.8063841133  1.5646605101 -0.0921562446
C   2.8790927224  1.0351814552  0.1391539862
C   2.0128468972 -1.620189182 -0.0409053412
C   1.4982261234  0.778098786  0.0324580247
C   1.0437000667 -0.5792230517 -0.0604418117
C   -2.6326989415 -0.0490332179 -0.2936398237
C   -3.9013756404 -0.2811289568 -0.4532963297
C   -4.9113461349 -0.5048382684  0.6524096259
H   4.8553392855  0.2155460661  0.2374818904
H   -0.6765435939 -1.8698182258 -0.2395840618
H   4.0799303168 -2.1410827918  0.0770188481
H   0.8675407771  2.853108177  0.0819526648
H   -1.5306383625  2.3701864706 -0.1064515651
H   3.2160416689  2.0645198702  0.2088617342
H   1.6747100557 -2.6487634924 -0.1110817195
H   -4.4434942211 -0.4503930677  1.6359354096
H   -5.3854318929 -1.4859720993  0.5454053367
H   -5.706649319  0.2460407347  0.6023461393
H   -4.3035465966 -0.3250115478 -1.4709133998
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
43.4020          77.4461          117.3978
143.8946          179.2768          213.0037
261.6343          341.6312          351.2802
399.1634          467.5913          486.6121
510.7458          524.2664          552.5185
627.9539          638.8825          677.8971
751.1375          759.4565          768.1959
773.3555          818.1814          839.1897
871.0952          877.9623          939.1176
953.0870          955.2411          979.1128
987.5019          1042.9277         1054.0182
1066.4858          1123.6996         1158.9187

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1170.9823          1177.3219          1220.1437
1263.2429          1288.4621          1323.3021
1345.9394          1373.0002          1400.4762
1409.9999          1451.5929          1471.3351
1485.2102          1492.3596          1517.6141
1563.9701          1621.3503          1632.9135
1908.4732          3018.4898          3030.1147
3068.4928          3117.0163          3156.3672
3158.9481          3162.0155          3174.7754
3178.2790          3188.4199          3189.4102
ZeroEnergy[kcal/mol] -45.94
ElectronicLevels[1/cm]      1
0 2
End
End
!-----
!-----well_i13-----
Well      i13
Species
RRHO
Geometry[angstrom]  24
C   3.6029795805 -0.1269478816 0.107728744
C   -0.4986047026 0.8190909805 -0.2780256337
C   3.2040079132 1.2081762145 -0.0805987972
C   -1.5338252759 -0.2171523031 -0.2067396262
C   0.2680364828 -1.8758306599 0.0836080401
C   -1.0445957716 -1.6002345685 -0.03169383
C   2.6439119896 -1.1329028773 0.1627618451
C   1.8687447557 1.5276286926 -0.2092203153
C   1.2823254272 -0.8438296835 0.0363930577
C   0.8629250269 0.5199561436 -0.1531969
H   4.6541220248 -0.3707866466 0.207807106
H   -0.811314682 1.8457408001 -0.4360746031
H   3.9525152017 1.9917147259 -0.1251291191
H   0.5944788765 -2.9030813786 0.2135501971
H   -1.7832100057 -2.3943596903 -0.0030686509
H   2.9497925334 -2.1646758189 0.3053099105
H   1.5646459273 2.5590706404 -0.3540673282
C   -3.4112884385 0.0332181973 -2.1037522386
C   -2.8301644552 -0.0001759359 -0.9214705655
C   -2.911122135 0.1540537564 0.5166084087
H   -2.8522750089 -0.1701877203 -3.0108056065
H   -4.4671248147 0.2649436354 -2.206583905
H   -3.3558239582 -0.6343452663 1.1168790595
H   -2.9684244912 1.1494996443 0.9466957506
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm]  66
53.4873          92.6295          177.3986
182.7825          233.7767          280.2562
362.8145          372.6432          412.2195
442.0220          466.4859          502.4190
510.5536          547.3933          617.3095

```

648.3904	668.9138	689.9380
719.1838	750.2947	757.7492
779.7213	801.5927	849.3599
863.9052	893.3926	921.5139
927.8405	933.0050	939.7836
974.4720	982.1289	1017.4368
1026.5969	1043.7682	1078.7331
1121.8761	1146.3172	1166.0118
1171.2531	1208.6799	1254.2587
1293.2818	1318.0808	1345.2619
1414.7238	1425.9777	1437.6208
1459.4771	1465.3239	1506.0680
1560.1938	1608.6869	1651.9473
1817.8471	3094.7741	3120.4536
3151.6867	3155.4207	3159.3249
3166.2944	3173.8913	3174.2490
3181.5657	3188.6372	3204.0166

ZeroEnergy[kcal/mol] -25.7

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----well_i14-----

Well i14

Species

RRHO

Geometry[angstrom] 24

C	-2.1708788549	-0.9260967149	-0.3726883959
C	1.0893593865	1.6631920972	0.4039510152
C	-2.4095324054	0.429497517	-0.04822489
C	2.3823548735	1.1992362363	0.3447741261
C	1.5648182311	-1.0121357589	-0.2392953773
C	2.6110617828	-0.1625122941	0.0134201264
C	-0.8849899129	-1.4061850374	-0.4371938672
C	-1.3588532039	1.2779392342	0.2054928637
C	0.2213700651	-0.556428538	-0.1807569801
C	-0.0191870874	0.8138277575	0.1475376935
H	-3.0086640883	-1.585144026	-0.5707759611
H	0.8975361375	2.7029599906	0.65215143
H	-3.4284324362	0.7971739777	-0.0006126874
H	1.7542526675	-2.0505915347	-0.491121139
H	3.6315121077	-0.5249128491	-0.0474037239
H	-0.6988288669	-2.4458287662	-0.6863204474
H	-1.5418755997	2.3182701253	0.4541486208
C	3.5587054705	2.1136065638	0.6502071931
C	5.8446403113	1.9199410102	-0.6014353623
C	4.5744444236	2.1773205664	-0.4187825047
H	3.1846346811	3.1215119617	0.8583038611
H	4.0529764614	1.7719585207	1.5773791701
H	6.4706545243	1.5275977338	0.2068777162
H	6.3419573316	2.0842372269	-1.5535534798

Core RigidRotor

SymmetryFactor 0.5

```

End
Frequencies[1/cm]   66
23.5293              71.2218              106.2674
179.2895             197.7096              241.6284
306.8364             324.0052              403.2800
406.3950             447.4936              487.0145
514.1745             526.7582              581.2887
636.3853             658.5397              735.8589
763.9667             781.1979              786.6345
832.6449             864.3947              878.5778
883.7540             889.7888              913.4227
947.6315             963.8884              977.5358
979.6539             996.2394             1042.1791
1042.5549            1147.5463             1172.2849
1177.9235            1188.0492             1204.4470
1237.0804            1277.1098             1288.2727
1303.1735            1391.7054             1396.5431
1406.7277            1413.4844             1447.3755
1474.0169            1502.4998             1545.8055
1612.3082            1645.6789             1673.1690
1734.1983            2923.2560             3025.6637
3044.3966            3148.0055             3152.9757
3157.0511            3158.8097             3162.5382
3174.7730            3178.2433             3187.6229
ZeroEnergy[kcal/mol] -36.53
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i15-----
Well      i15
Species
RRHO
Geometry[angstrom]   24
C   -3.6853081126  0.3132365987  0.1702103376
C    0.3608289559 -0.8464602687 -0.331969764
C   -3.3694510029 -1.0152460623 -0.1960618228
C    1.3966585044  0.0491667037 -0.14136726
C   -0.2546159212  1.8011835045  0.3969886337
C    1.005369486  1.3450591001  0.2165516366
C   -2.6855099659  1.2359034637  0.3652824467
C   -2.0597060833 -1.3964940546 -0.3597603906
C   -1.3247278148  0.8732493513  0.2031617884
C   -1.0000621699 -0.4714203142 -0.1676652918
C    2.8527805263 -0.3334369186 -0.3291945064
C    3.9744330945 -0.6029692777 -2.5658237144
C    3.4180528077  0.1662710387 -1.6360944049
H   -4.7226549234  0.6021367903  0.2969927092
H    0.5871443192 -1.8713395262 -0.6141663866
H   -4.1673864743 -1.7333902279 -0.3472912581
H   -0.4728050859  2.8260688121  0.680144627
H   -2.9258272111  2.2558780549  0.6463617595
H   -1.8173984251 -2.4161315094 -0.6407623727

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H   3.4330494535  0.091660233  0.4985215128
H   2.9570784298 -1.4202179574 -0.2727942107
H   4.0594557285 -1.6784160801 -2.4402428471
H   4.3673190168 -0.1865484719 -3.4864509305
H   3.3445228682  1.2394080179 -1.7995902909
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
23.6820           59.0243           101.6365
181.5633          191.6930           248.0398
317.3843          372.9903           397.9920
411.1026          476.6877           480.2778
530.8658          541.4642           617.4221
633.9593          657.9506           746.8350
762.7680          766.9880           777.8534
838.1710          870.9931           875.9615
894.8381          935.2553           940.2048
949.8672          954.7086           964.7459
994.1871          1032.2668          1041.9649
1106.3999          1148.5986          1169.3863
1180.3087          1217.6022          1222.1123
1253.9220          1275.1993          1310.5901
1325.9500          1342.1294          1387.3455
1399.3607          1432.6102          1453.6459
1473.9690          1479.0407          1528.4245
1595.7633          1626.4345          1655.7364
1705.8503          3015.9238          3072.6714
3123.8773          3134.8424          3144.8492
3157.3214          3158.6700          3163.8622
3175.8249          3188.2097          3209.2217
ZeroEnergy[kcal/mol] -32.01
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i16-----
Well      i16
Species
RRHO
Geometry[angstrom]  24
C   -3.7134868502  0.4626528905  0.2739172892
C    0.214288241 -1.0043733187 -0.0577859539
C   -3.494811008 -0.9322214027  0.3574026028
C    1.3142881011 -0.2303580259 -0.2438987554
C   -0.20765562  1.6827450688 -0.2205981714
C    1.0628592481  1.1754979655 -0.3286915892
C   -2.6583811093  1.3234110898  0.0870521733
C   -2.2252660656 -1.4470199529  0.2526507402
C   -1.3319692981  0.835237156 -0.0255415656
C   -1.1155562205 -0.5842220609  0.0596164515
H   -4.7219473444  0.851509706  0.3586365615
H   -4.3380476807 -1.5973856008  0.5053309714

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H   -0.3701676676  2.7532198088 -0.2890533193
H   1.9037839135  1.8457739559 -0.4828550945
H   -2.8279753478  2.3935127984  0.0230310287
H   -2.0501141594 -2.514519772  0.3160451783
H   2.3223365968 -2.4955322298 -1.654109045
C   2.7280854243 -0.7750165058 -0.3358122069
C   3.3978033994 -3.1730374526  0.0059400542
C   2.8010804537 -2.2288520731 -0.7140786691
H   3.276661245 -0.1786533269 -1.0765969219
H   3.2394342126 -0.6177228668  0.6213419624
H   3.8776145937 -2.9485565711  0.9539739199
H   3.4273659427 -4.20543428 -0.3236126411
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
29.4750           63.7939           98.6585
154.7319          180.3027          259.2692
303.6574          371.7089          408.3747
432.7212          474.9463          502.2206
509.5688          520.0494          613.6675
626.7124          648.4669          742.2549
755.5953          771.3618          779.8885
815.5489          875.6975          903.4153
928.6905          943.7640          951.9850
958.1390          969.3808          974.3603
997.1942          1029.9790         1039.7471
1127.6701         1139.4412         1161.7711
1171.0638         1195.6947         1236.1080
1245.6112         1265.1242         1311.1170
1325.8133         1359.6068         1364.7015
1394.7834         1447.4229         1450.8237
1471.1123         1496.4028         1520.5586
1583.0241         1643.1138         1664.7373
1709.9389         3001.8781         3033.6926
3124.0430         3133.4331         3146.7504
3157.4233         3168.5484         3172.1509
3181.6314         3191.7745         3209.6418
ZeroEnergy[kcal/mol] -31.49
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----well_i17-----
Well      i17
Species
RRHO
Geometry[angstrom]  24
C   3.7558777361 -0.0540624488  0.3680328436
C   -0.3416996382 -0.7685246127 -0.4463485298
C   3.3030906976 -1.3720213857  0.1260750898
C   -1.216707186  0.2870671651 -0.4720146886
C   0.5608043689  1.8583828  0.0358069038

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C   -0.7618178876  1.611174834 -0.2290842351
C   2.8721260868  0.9971502426  0.3402203165
C   1.9763841959 -1.6101524827 -0.1384665874
C   1.4941543391  0.7879163108  0.0701566683
C   1.0352441678 -0.5478781782 -0.1750846005
C  -2.7093623931  0.2752732546 -0.7383053172
C  -1.9121632934  2.59519271 -0.3129352415
C  -3.0893650794  1.7217014013 -0.6289583335
H   4.8052619337  0.1227704547  0.5758652948
H  -0.6837840657 -1.7825540832 -0.6313961324
H   4.009143534 -2.1945588955  0.1504175309
H   0.9140986772  2.8683126525  0.2222260121
H   3.2183818029  2.0088651526  0.525735636
H   1.6277763572 -2.6210058112 -0.32427399
H  -2.9431969492 -0.1491363648 -1.727291071
H  -3.2470865904 -0.3582004996 -0.0155048744
H  -1.7366498704  3.3620844441 -1.0836504992
H  -2.0408605404  3.152806685  0.6280032609
H  -4.0973234032  2.0920946549 -0.7594894562
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
94.3256           122.3123           152.5677
256.8166          258.4568           286.3775
366.4610          404.7816           405.2049
411.6028          486.6988           535.1487
575.3483          629.0985           649.8059
718.4084          724.6065           756.7602
779.4559          785.5189           829.0436
858.7876          869.9437           889.3510
912.8743          920.9225           929.0231
942.2427          965.1186           992.4063
1025.1768         1042.2542          1088.4897
1133.7233         1134.6911          1168.5879
1172.1536         1181.5257          1222.9891
1245.4172         1265.9690          1283.2206
1308.2046         1349.1397          1368.7828
1392.9369         1418.0195          1455.5254
1459.8124         1485.0784          1487.7814
1537.5065         1614.4639          1652.0068
1678.1141         2954.9278          2958.3026
2959.3328         2959.3826          3152.4401
3154.2132         3155.7817          3160.5562
3173.3421         3186.4986          3204.3097
ZeroEnergy[kcal/mol] -65.35
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----well_i18-----
Well      i18
Species

```

```

RRHO
Geometry[angstrom]    24
C   -3.607062069 -0.4605740743 -0.0318252876
C    0.6292210744 -0.3906776281  0.0277618079
C   -2.8882487414 -1.6773337816 -0.046284512
C    1.2868335286  0.8210121746  0.0610070201
C   -0.805030168  2.0109928583  0.0561101079
C    0.5683326982  2.036618594  0.0754479664
C   -2.9353082483  0.7377778544  0.0013687349
C   -1.5135397761 -1.6733497794 -0.0272977677
C   -1.5174417576  0.7812486353  0.0217280292
C   -0.7887686853 -0.4535965745  0.0070463758
C    2.7894119791  0.6349755857  0.0776853037
C    1.6080635607 -1.5476234172  0.0179128255
C    2.9386691442 -0.8562776438  0.0494437806
H   -4.6910512064 -0.4770673972 -0.0470524222
H   -3.4275925484 -2.617699124 -0.072494086
H   -1.3698888888  2.9374094166  0.0668786518
H    1.0981762608  2.9832118707  0.1016345141
H   -3.4852400794  1.6733450155  0.0125482626
H   -0.9695478063 -2.6110225926 -0.0385263585
H    3.2723483421  1.1276919034 -0.7815371326
H    3.2485491479  1.0920899577  0.9690463158
H    1.4599913509 -2.2199256023  0.87850768
H    1.4834254148 -2.1853272914 -0.8721972472
H    3.8892594724 -1.3724059599  0.0520514372
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]    66
107.0698           128.5708           178.4724
225.9664           235.7410           276.7820
353.3120           420.6603           428.3135
460.9729           507.0879           519.1917
533.6427           603.8140           642.7945
671.0885           744.3922           751.3863
781.2880           788.6778           819.8450
868.7788           873.0729           911.2819
928.9227           930.0882           958.7208
960.1594           970.2790           993.5074
1025.4853          1045.3607          1072.8194
1129.5222          1137.3259          1167.6873
1177.4641          1184.1963          1212.0690
1234.2226          1271.5683          1283.4381
1324.5049          1346.0158          1377.9853
1400.1540          1412.7110          1457.5895
1463.8005          1470.8255          1497.5447
1552.7075          1612.0443          1636.1373
1665.6815          2948.0004          2950.1224
2952.4369          2952.5572          3155.2200
3157.3450          3165.1983          3173.9764
3178.2905          3188.1393          3204.5390
ZeroEnergy[kcal/mol] -66.0
ElectronicLevels[1/cm]    1

```

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0 2
End
End
!-----
!-----well_i19-----
Well      i19
Species
RRHO
Geometry[angstrom] 24
C 3.6318810329 0.4807542745 0.0164837667
C -0.2434383243 -1.2107040763 0.1715009654
C 3.4731057942 -0.897396964 0.2869243159
C -1.3837031239 -0.4316568618 -0.0393356273
C 0.0552111971 1.5277580953 -0.330193233
C -1.1903361535 0.9723244628 -0.2716870932
C 2.5285366997 1.2777531678 -0.1910255182
C 2.2177639331 -1.4537653676 0.3414043115
C 1.2231825373 0.7358196657 -0.1410187339
C 1.0581642944 -0.660774276 0.1251246419
H 4.6272643362 0.9083445479 -0.0243518639
H -0.3439809883 -2.2578012139 0.424775612
H 4.3486207288 -1.5151830757 0.4522842615
H 0.1703771649 2.5900976259 -0.5195887297
H -2.066656421 1.5949285609 -0.4185021695
H 2.6483304895 2.3369353075 -0.3945287055
H 2.0951971186 -2.5116851041 0.5493027687
C -2.7325403717 -0.9266761192 0.0003385113
C -2.5849411392 -3.3960708672 -0.4579690801
C -3.2260580323 -2.2484996023 -0.0851142619
H -3.4928412555 -0.1568802084 0.1001777134
H -3.1214040518 -4.3366536794 -0.4808369014
H -1.5578416823 -3.4130030955 -0.7959543381
H -4.2868677829 -2.3439631969 0.1390253873
Core RigidRotor
SymmetryFactor 0.5
End
Frequencies[1/cm] 66
58.9015 101.5076 129.9387
189.0148 215.3316 278.4754
332.1181 389.6537 410.0791
432.0402 481.8984 523.5196
526.6313 569.6826 605.0500
646.2998 656.8319 739.4751
751.9518 773.1264 779.2752
794.0026 833.6479 854.9327
873.1235 906.7269 924.4219
961.5779 965.1367 978.2899
991.8832 993.5742 1020.8295
1042.5393 1112.0085 1153.8579
1171.0841 1179.3984 1211.4510
1229.4784 1267.6219 1286.0095
1293.7944 1367.4051 1389.9154
1411.1832 1442.4774 1453.8730
1478.7488 1489.1216 1534.9779

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1561.9633          1592.1557          1632.4830
1651.8740          3119.1245          3145.6842
3154.2215          3155.9985          3157.5469
3161.9987          3174.4123          3175.3508
3187.9911          3197.8435          3243.0872
ZeroEnergy[kcal/mol] -62.2
ElectronicLevels[1/cm]      1
0  2
End
End
!-----
!-----well_i20-----
Well      i20
Species
RRHO
Geometry[angstrom]      24
C   3.6230700817  0.4619957723 -0.0842389153
C   -0.3031069253 -1.2250619843  0.5110391305
C   3.4846128781 -0.9173547634  0.0738051482
C   -1.4265864514 -0.345334985  0.002846485
C   0.0309431114  1.564962644 -0.0513082859
C   -1.2438720213  1.0249336922 -0.1416123886
C   2.4972689638  1.2729330543 -0.0993943822
C   2.2137579479 -1.4728422414  0.2311596715
C   1.205775024  0.7294117857  0.0451732
C   1.0745113243 -0.6742348158  0.2252395833
C   -2.5378683456 -1.184410105 -0.3056176019
C   -0.6972323073 -2.6447765608  0.0209552627
C   -2.171488828 -2.4938495309 -0.2745764711
H   4.6079761391  0.9004444951 -0.2002591312
H   -0.4108451995 -1.2340230922  1.6114296777
H   4.3598001422 -1.5570681438  0.0808093914
H   0.1760726786  2.6330330374 -0.1708482773
H   -2.0855113347  1.6644272303 -0.3897136437
H   2.6027307471  2.3442710184 -0.2374252175
H   2.11440712 -2.544390969  0.3699087987
H   -3.5226658597 -0.8182249332 -0.5708291764
H   -0.4824639782 -3.4278222972  0.7536584406
H   -0.1496975418 -2.9074488569 -0.8955033665
H   -2.8191913655 -3.3310424509 -0.5025069317
Core RigidRotor
SymmetryFactor  0.5
End
Frequencies[1/cm]  66
95.7042          110.4329          211.0156
234.1449          251.2703          394.0126
415.9914          425.1121          437.8193
504.0759          519.7746          539.3193
604.9982          654.0605          690.8255
716.1939          724.9124          750.4712
775.3882          796.1987          814.4065
859.2284          880.9569          921.4952
924.5328          946.7092          948.3532
952.4561          979.6145          983.2397

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1024.6200	1058.9219	1095.7327
1118.8624	1139.2165	1159.6583
1180.5462	1216.7607	1227.0960
1238.9974	1247.5655	1282.7061
1298.3331	1315.9616	1321.0889
1345.9526	1387.8781	1407.0705
1463.7064	1481.3539	1511.7609
1531.3195	1551.4635	1600.2444
1630.8057	2899.7681	2988.1683
3058.2107	3152.5933	3155.1394
3160.4981	3172.3421	3174.9839
3181.3335	3186.8673	3203.2937

ZeroEnergy[kcal/mol] -64.72

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----c10h7_c3h4_p0p-----

Bimolecular p0p

Fragment c3h4

RRHO

Geometry[angstrom] 7

C	-0.823420841	0.0519880348	-0.0208571707
C	1.824711204	-0.1816552298	0.0001678957
H	-1.8820502847	0.1362504236	-0.0342313517
H	2.1265806386	-1.2327357481	0.0038417281
H	2.2515118512	0.2935470245	0.887798287
H	2.2667123243	0.2920674571	-0.8807572055
C	0.3727611076	-0.0556769621	-0.0121801829

Core RigidRotor

SymmetryFactor 3.0

End

Frequencies[1/cm] 15

339.4278	339.9763	666.0166
666.0469	943.1202	1056.2902
1056.6567	1416.3162	1479.4028
1479.6937	2229.8067	3026.9185
3085.7411	3086.1443	3478.9987

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 1

End

Fragment c10h7

RRHO

Geometry[angstrom] 17

C	-2.342087	-0.789687	0.000182
C	1.23599	1.492987	-0.00007
C	-2.406991	0.622556	-0.000082
C	2.395952	0.795395	-0.00008
C	1.355609	-1.327182	0.000189
C	2.524369	-0.593594	0.000023
C	-1.124987	-1.426414	-0.000392
C	-1.255124	1.371674	0.000158

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C    0.086626 -0.68687 -0.00012
C    0.017308 0.74503 0.000139
H   -3.258566 -1.368743 0.000087
H    1.201705 2.577724 -0.00028
H   -3.373351 1.114428 0.000661
H    1.39504 -2.412201 0.000526
H    3.493202 -1.079675 0.000221
H   -1.073657 -2.510327 -0.000363
H   -1.30436 2.455421 -0.000531
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  45
174.5523          191.9823          368.8691
386.9856          471.7499          485.5864
511.3155          520.6059          611.1652
628.1914          745.0901          754.9555
767.1418          793.9645          805.9451
845.2289          888.1353          936.1904
956.7704          970.6818          996.7989
1040.0912         1049.2482         1141.2669
1161.1784         1172.2344         1208.1577
1250.0871         1276.7535         1334.8589
1385.5649         1394.0363         1457.0524
1468.7884         1530.4230         1592.5026
1620.1890         1656.5683         3155.0771
3158.4833         3159.6258         3164.2142
3175.9226         3179.5633         3188.1262
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0 2
End
GroundEnergy[kcal/mol] 0.0
End
!-----c10h7_c3h4_p0a-----
Bimolecular  p0a
Fragment      c3h4
RRHO
Geometry[angstrom]  7
C   -0.7953643067 0.0340930197 0.0003929351
C    1.7999079767 -0.188313622 -0.0384040502
H   -1.2789000818 0.9884787247 0.182918491
H   -1.4365104427 -0.8255826572 -0.1664284561
H    2.3603730273 -0.4130354538 0.8635083944
H    2.3636835038 -0.0613232862 -0.9572540549
C    0.5024913234 -0.0757887252 -0.0189202593
Core RigidRotor
SymmetryFactor 4.0
End
Frequencies[1/cm]  15
371.2233          371.5183          865.8663
866.2617          884.0403         1016.3687
1016.5866         1109.0953         1422.1712
1479.1925         2051.9260         3118.9601

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3123.0938          3193.6015          3194.4729
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment      c10h7
RRHO
Geometry[angstrom]  17
C   -2.342087 -0.789687 0.000182
C   1.23599 1.492987 -0.00007
C   -2.406991 0.622556 -0.000082
C   2.395952 0.795395 -0.00008
C   1.355609 -1.327182 0.000189
C   2.524369 -0.593594 0.000023
C   -1.124987 -1.426414 -0.000392
C   -1.255124 1.371674 0.000158
C   0.086626 -0.68687 -0.00012
C   0.017308 0.74503 0.000139
H   -3.258566 -1.368743 0.000087
H   1.201705 2.577724 -0.00028
H   -3.373351 1.114428 0.000661
H   1.39504 -2.412201 0.000526
H   3.493202 -1.079675 0.000221
H   -1.073657 -2.510327 -0.000363
H   -1.30436 2.455421 -0.000531
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  45
174.5523          191.9823          368.8691
386.9856          471.7499          485.5864
511.3155          520.6059          611.1652
628.1914          745.0901          754.9555
767.1418          793.9645          805.9451
845.2289          888.1353          936.1904
956.7704          970.6818          996.7989
1040.0912         1049.2482         1141.2669
1161.1784         1172.2344         1208.1577
1250.0871         1276.7535         1334.8589
1385.5649         1394.0363         1457.0524
1468.7884         1530.4230         1592.5026
1620.1890         1656.5683         3155.0771
3158.4833         3159.6258         3164.2142
3175.9226         3179.5633         3188.1262
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol]  1.1
End
!-----h_c10h6_p1-----
Bimolecular    p1
Fragment      c10h6
RRHO

```

```

Geometry[angstrom]    23
C   -3.4297275383  0.6926828295  0.0039083678
C    0.2561865651 -1.4034018581 -0.0085023831
C   -3.4192071452 -0.7206557811 -0.0006487593
C    1.4301622887 -0.6884204437 -0.0080385742
C    0.2375332283  1.4304945887  0.0005892895
C    1.4176697405  0.7420283073 -0.0034772169
C   -2.2463676634  1.3923572342  0.0043120379
C   -2.2271153712 -1.4039826096 -0.0046946993
C   -0.9977522925  0.720531113  0.0002165193
C   -0.9860464949 -0.7144502301 -0.0044032352
C    2.8281081359 -1.1220833093 -0.0116269207
C    2.8483269174  1.2348432817 -0.004056437
C    3.6409965108 -0.0519460444 -0.0095010525
H   -4.3754448604  1.222915632  0.0070883174
H    0.2599391198 -2.4888289276 -0.0119952953
H   -4.3573702871 -1.2643043552 -0.0009374379
H    0.217623734  2.5163608324  0.0041197655
H   -2.2529829395  2.477688416  0.0078122976
H   -2.2185160279 -2.4892073171 -0.0081914894
H    3.1434835396 -2.157922306 -0.0153885217
H    3.0748527551  1.8496933954  0.8759822814
H    3.072160391  1.8553276045 -0.8808330576
H    4.7229266941 -0.0789710526 -0.0107867963
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]    63
102.2294             134.8645             251.8437
263.5800             278.6570             394.6986
405.8898             417.1671             426.3605
487.3719             559.6989             578.1974
628.8197             686.4746             732.6775
738.6653             751.4693             764.7804
783.4099             806.1723             857.4753
858.7720             890.3014             902.4118
913.7707             955.6878             957.5792
963.1137             970.5211             991.6628
1043.4534            1077.4282            1121.2771
1155.6730            1169.2853            1174.4788
1180.6497            1244.5385            1251.5039
1268.6960            1282.1901            1347.9739
1373.3697            1387.7710            1434.9787
1446.5223            1470.3410            1486.9167
1537.3526            1611.9868            1627.0456
1655.0763            1677.6805            3013.8854
3035.4208            3153.1920            3155.6051
3159.0651            3162.4123            3173.3962
3186.6618            3189.2638            3212.1926
ZeroEnergy[kcal/mol]    0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment              H

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Atom
Mass[amu]      1
ElectronicLevels[1/cm]      1
0      2
End
GroundEnergy[kcal/mol] -36.51
End
!-----h_c10h6_p2-----
Bimolecular    p2
Fragment       c10h6
RRHO
Geometry[angstrom]      23
C   3.3470139691 -0.1784239349 -0.001643978
C   -0.8842205267 -0.4325083205 -0.0072564037
C   2.726429771 -1.4486079448 -0.0077584959
C   -1.6327602416 0.7404671779 -0.0032145561
C   0.3640781219 2.0708040892 0.0046323389
C   -1.0114628758 2.0005023316 0.0027143091
C   2.5833180704 0.9631720545 0.0024139944
C   1.355902182 -1.5520334827 -0.0096475295
C   1.165120296 0.8966729154 0.0005939313
C   0.537531976 -0.3935695503 -0.0055813048
C   -3.0990961767 0.3869034187 -0.0067243045
C   -1.8099242179 -1.5696327613 -0.0128348109
C   -3.0780386636 -1.1207224362 -0.0124526263
H   4.4290830247 -0.1096456294 -0.0001791325
H   3.3379375392 -2.3440222559 -0.0109806364
H   0.860868578 3.0352454583 0.0093447647
H   -1.6062808473 2.908085251 0.0057784256
H   3.0580407341 1.9390508141 0.007080557
H   0.8891185 -2.5303532928 -0.01442073
H   -3.6221352851 0.7853374153 0.8721696031
H   -3.6190854475 0.7919835703 -0.8844308124
H   -1.5129772577 -2.6101143399 -0.0173138716
H   -3.9711972226 -1.7309105476 -0.0167237316
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]      63
113.5257      131.9163      229.2535
241.8649      268.1291      387.6530
432.9010      438.9526      463.5719
506.1584      519.7956      565.0100
613.2436      666.3208      682.0518
723.0441      748.4811      753.1903
798.3278      817.3537      841.0725
879.0965      882.4712      933.2309
950.4010      954.8911      958.7597
966.8124      969.3282      992.8559
1043.9091     1074.2166     1126.1545
1143.1105     1166.9833     1178.4415
1192.0183     1216.8068     1236.5320
1283.2710     1293.5284     1351.7454
1378.3222     1389.1206     1430.1706

```

1431.5184	1469.3722	1486.3917
1555.1522	1584.8304	1618.8469
1634.2323	1664.3623	3014.4097
3037.1196	3155.8991	3157.6508
3165.4471	3174.7872	3178.0459
3188.0059	3195.5734	3217.7099

```

ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment      H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]    1
0 2
End
GroundEnergy[kcal/mol] -36.19
End
!-----h_c10h6_p3-----
Bimolecular  p3
Fragment      c10h6
RRHO
Geometry[angstrom]      23
C   3.3589805782 -0.1589532841 -0.0052741521
C   -0.8626124942 -0.4592216299 0.0061451685
C   2.7512244302 -1.4362419127 -0.0057558711
C   -1.6304316353 0.7002778521 0.0104255245
C   0.3504445096 2.0582620245 0.0073112859
C   -1.0208972146 1.9753841923 0.0110703316
C   2.58240266 0.9743296087 -0.0010636067
C   1.3828455855 -1.5556845697 -0.0020600345
C   1.1658232353 0.8928735063 0.0028576508
C   0.5497812064 -0.4047593755 0.0022898527
C   -3.0471181043 0.3231433831 0.013518318
C   -1.786615793 -1.65287093 0.0068930735
C   -3.1559300206 -1.0165005908 0.0115352725
H   4.4401442599 -0.0787740034 -0.00823888
H   3.372925776 -2.3247255603 -0.0090822067
H   0.8378607683 3.0277237362 0.0077226495
H   -1.6280620211 2.8741736402 0.0144845493
H   3.0467756867 1.9552584003 -0.0006703734
H   0.9246806356 -2.5385591873 -0.0024656456
H   -3.8673579721 1.0301984874 0.0178637838
H   -1.6405804813 -2.2929696258 -0.8725833972
H   -1.6357579267 -2.2952054346 0.8839587431
H   -4.0761106684 -1.5851637269 0.0138329637
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  63
111.6057           140.7443           235.7064
237.2840           257.3698           398.3460
432.9203           435.8184           465.2515
517.6631           520.4055           551.8391

```

616.8391	670.8841	681.8888
717.6433	751.4780	760.5919
787.6060	828.8756	839.7089
870.5955	872.9566	937.1401
954.7419	955.4339	959.8592
969.6851	982.2343	991.7663
1043.6091	1060.8926	1117.9424
1144.2864	1166.9366	1179.2631
1185.6203	1233.5150	1244.7639
1263.9305	1288.3090	1363.9889
1378.3244	1398.4726	1416.6215
1434.3888	1470.0882	1487.4172
1552.8699	1587.7715	1621.6410
1637.3459	1664.1362	3014.2828
3037.1636	3156.0941	3158.7295
3163.7980	3176.1937	3177.0078
3187.4191	3190.5460	3215.9190
ZeroEnergy[kcal/mol]	0.0	
ElectronicLevels[1/cm]	1	
0 1		
End		
Fragment	H	
Atom		
Mass[amu]	1	
ElectronicLevels[1/cm]	1	
0 2		
End		
GroundEnergy[kcal/mol]	-36.33	
End		
!-----h_c10h6_p4-----		
Bimolecular	p4	
Fragment	c10h6	
RRHO		
Geometry[angstrom]	23	
C	3.7695852196 -0.0064018801 0.1624634079	
C	-0.3681027934 -0.8226648439 -0.1754219653	
C	3.3187500647 -1.3444696048 0.0757045779	
C	-1.2899850887 0.2105062445 -0.2022003511	
C	0.51585409 1.8271389281 -0.004209719	
C	-0.8220659745 1.5561515634 -0.1137952259	
C	2.8687958828 1.0311253417 0.1375131586	
C	1.9775783278 -1.6190602397 -0.0341907195	
C	1.4774799929 0.7826568887 0.0249353278	
C	1.0200273942 -0.5701457584 -0.0628983946	
C	-2.6885215071 -0.0499966899 -0.3160526462	
C	-3.8738171039 -0.2543236385 -0.412071668	
C	-5.3035998711 -0.5068617608 -0.5273154055	
H	4.8310747361 0.1965152437 0.2488677317	
H	-0.7141061282 -1.8479727961 -0.2418500721	
H	4.0392322254 -2.154399737 0.0964489004	
H	0.8579800055 2.8547663717 0.0622144114	
H	-1.5472635443 2.3605226794 -0.1350036066	
H	3.2126102001 2.0581942628 0.2039493882	
H	1.6305100804 -2.6449192567 -0.1008133461	

```

H   -5.7209994588 -0.8553331929 0.4225559236
H   -5.5092767819 -1.2719180664 -1.2819815849
H   -5.8417039676 0.4008889412 -0.8153441225
Core  RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]  63
13.2466           62.5761           74.7243
164.4456          182.3529          269.4018
284.4434          345.5747          373.0123
393.0782          436.4623          485.1788
515.9132          552.1632          557.9209
616.2315          658.6678          661.8111
760.2520          779.5747          781.0217
833.6909          858.7340          874.8436
913.6325          952.6072          964.9148
979.7661          996.7664         1014.7086
1042.2834         1049.7956         1054.1792
1152.0061         1172.8489         1178.1938
1211.5509         1249.9931         1286.9966
1298.8516         1371.5645         1395.9116
1403.2038         1416.5169         1464.4389
1478.0379         1479.1806         1502.0790
1537.4508         1603.0487         1641.3785
1666.7591         2336.3606         3019.6932
3073.9064         3079.7539         3157.6695
3161.4205         3163.8674         3175.3187
3178.1638         3188.2924         3191.9414
ZeroEnergy[kcal/mol]  0.0
ElectronicLevels[1/cm]  1
0  1
End
Fragment          H
Atom
Mass[amu]  1
ElectronicLevels[1/cm]  1
0  2
End
GroundEnergy[kcal/mol] -9.62
End
!-----h_c10h6_p5-----
Bimolecular  p5
Fragment      c10h6
RRHO
Geometry[angstrom]  23
C           3.674981      0.497930     -0.000270
C          -0.219804     -1.159771      0.000398
C           3.507073     -0.905745     -0.000471
C          -1.335316     -0.344858      0.000639
C           0.104371      1.613217      0.000265
C          -1.150805      1.068039      0.000508
C           2.577411      1.326248     -0.000042
C           2.247044     -1.454470     -0.000300
C           1.265061      0.792212      0.000092

```

C	1.093658	-0.627265	0.000071
C	-2.678275	-0.945911	0.000639
C	-4.953878	0.338200	-0.001024
C	-3.818184	-0.297671	-0.000173
H	4.674304	0.918331	-0.000291
H	-0.342425	-2.238727	0.000371
H	4.379634	-1.549380	-0.000766
H	0.228583	2.691348	0.000169
H	-2.024495	1.709749	0.000604
H	2.703431	2.404084	0.000102
H	2.118144	-2.531928	-0.000473
H	-2.716374	-2.033955	0.001034
H	-5.449819	0.614651	-0.927951
H	-5.451004	0.614896	0.925210

Core RigidRotor
SymmetryFactor 1.0
End

Frequencies[1/cm] 63

46.2339	103.8385	125.7138
182.5167	253.5967	276.1306
328.7230	379.4763	401.6511
411.5401	480.6687	497.2674
525.9436	594.2023	604.9617
644.7759	684.6387	761.7100
766.4329	782.3325	784.1895
836.0403	872.7358	881.4050
888.9360	896.1518	922.2063
963.8350	967.0643	983.3427
995.5075	1012.7378	1042.5921
1102.8136	1151.4380	1174.0129
1179.9562	1197.0911	1240.8038
1280.4937	1289.0527	1327.6220
1393.1879	1397.8004	1412.9141
1461.6268	1483.9705	1506.4370
1544.0494	1609.8810	1643.4084
1667.4288	2033.5041	3102.7160
3118.8576	3154.6031	3157.3764
3159.5801	3162.9618	3171.8426
3174.7675	3182.2671	3187.6613

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End

Fragment H
Atom
Mass[amu] 1
ElectronicLevels[1/cm] 1
0 2
End

GroundEnergy[kcal/mol] -7.24
End

!-----h_c10h6_p6-----
Bimolecular p6
Fragment c10h6

```

RRHO
Geometry[angstrom] 23
C -3.601815 0.383900 0.302093
C 0.331336 -1.086775 -0.247675
C -3.363878 -1.009966 0.307200
C 1.382170 -0.220264 -0.431775
C -0.134704 1.666895 -0.258174
C 1.134016 1.177774 -0.433294
C -2.561681 1.263041 0.118863
C -2.091489 -1.497572 0.129425
C -1.236971 0.792021 -0.067861
C -0.995906 -0.616759 -0.062344
C 2.794036 -0.741286 -0.658787
C 4.583078 0.196625 1.078480
C 3.776591 -0.228610 0.296433
H -4.610267 0.755805 0.444027
H 0.506299 -2.158545 -0.239833
H -4.192432 -1.694002 0.452640
H -0.311403 2.737565 -0.261235
H 1.966220 1.860584 -0.565497
H -2.741326 2.333194 0.115215
H -1.908480 -2.567183 0.133933
H 2.788502 -1.834732 -0.616378
H 3.120378 -0.476294 -1.672758
H 5.293819 0.569455 1.774398
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 63
21.6630 74.6359 142.6424
180.7269 243.9161 286.6814
331.4442 373.4920 402.0165
408.0951 485.4417 503.1293
526.7069 576.4951 635.5364
658.0474 667.8370 678.5675
737.5344 764.6428 781.4020
786.3882 832.1626 868.5120
878.8089 903.6712 946.9423
958.7772 965.8670 979.7131
985.0094 996.4644 1042.5726
1148.0008 1172.5342 1179.0625
1188.9602 1216.9373 1239.4898
1277.2317 1289.1479 1325.1916
1392.2986 1396.8940 1408.1882
1466.5377 1474.9665 1503.1218
1545.9904 1612.9193 1646.3300
1674.0852 2223.3362 3008.3643
3056.3908 3153.8497 3157.5197
3159.6598 3162.9819 3175.1434
3179.1100 3187.9599 3476.1676
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 1
End

```

```

Fragment      H
Atom
Mass[amu]      1
ElectronicLevels[1/cm]      1
0      2
End
GroundEnergy[kcal/mol] -2.25
End
!-----ch3_c12h8_p7-----
Bimolecular      p7
Fragment      c12h8
RRHO
Geometry[angstrom]      20
C      3.236624      0.172310      0.00
C      -0.841043      -0.948009      0.00
C      2.881179      -1.197039      0.00
C      -1.833267      0.017271      0.00
C      -0.145939      1.764012      0.00
C      -1.464948      1.395382      0.00
C      2.263177      1.142223      0.00
C      1.559667      -1.569997      0.00
C      0.889207      0.791807      0.00
C      0.528778      -0.592960      0.00
C      -4.379851      -0.646290      0.00
C      -3.212685      -0.349389      0.00
H      4.283729      0.453226      0.00
H      -1.115580      -1.996676      0.00
H      3.659088      -1.952091      0.00
H      0.123389      2.814985      0.00
H      -2.247821      2.143774      0.00
H      2.535296      2.192583      0.00
H      1.284563      -2.619418      0.00
H      -5.408056      -0.912317      0.00
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm]      54
      87.9880      133.1440      181.2468
      218.2255      352.1262      383.4870
      401.5587      429.5214      484.5990
      516.8219      552.4624      559.6133
      629.3281      632.9808      663.6020
      685.9742      691.9308      760.9473
      779.8212      780.6114      834.1419
      876.3712      899.3207      915.5693
      966.6536      971.2117      980.9216
      999.0278      1041.9866      1145.5746
      1172.8883      1177.9761      1185.7844
      1233.3388      1277.2123      1289.8811
      1371.2885      1395.2179      1403.3569
      1465.1985      1499.2505      1537.6500
      1603.6481      1640.9279      1667.3435
      2205.9189      3158.8057      3163.5226
      3165.7769      3176.3887      3179.5926

```

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3189.0981          3194.5312          3477.6126
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
Fragment      ch3
RRHO
Geometry[angstrom]      4
C      0.000000      0.0000      0.000
H      -0.9358075      -0.5401365      0.000
H      0.9358075      -0.5401365      0.000
H      0.0000      1.080495      0.000
Core  RigidRotor
SymmetryFactor 6.0
End
Frequencies[1/cm]  6
  505.5776          1403.1131          1403.3797
 3103.7859          3282.6714          3283.0465
ZeroEnergy[kcal/mol]      0.0
ElectronicLevels[1/cm]    1
0 1
End
GroundEnergy[kcal/mol] -15.3
End

```

```

!-----bar_ts0-1-----
Barrier      ts0-1  i1  p0p
RRHO
Geometry[angstrom]      24
C   3.76994   0.01624   0.41853
C  -0.28693  -0.8287   -0.49631
C   3.3644   -1.31764   0.18061
C  -1.14991   0.2194   -0.55546
C   0.52793   1.82404  -0.02216
C  -0.79045   1.55162  -0.31983
C   2.85519   1.03897   0.35397
C   2.05341  -1.60222  -0.11632
C   1.49237   0.78284   0.04936
C   1.08338  -0.56924  -0.19119
H   4.80736   0.22767   0.65208
H  -0.60794  -1.85086  -0.67459
H   4.09504  -2.1172   0.23374
H   0.84704   2.84558   0.16309
H  -1.52524   2.3479  -0.37143
H   3.16487   2.06311   0.5357
H   1.7413   -2.62538  -0.29887
C  -3.41112  -0.22226  -1.06748
C  -4.62584  -0.43934   1.2916
C  -4.0514   -0.33822  -0.04039
H  -3.17228  -0.18452  -2.10395
H  -5.38494   0.33146   1.45299
H  -3.85218  -0.31702   2.05762
H  -5.09881  -1.41373   1.44402
Core  RigidRotor

```

```

SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  290.3817
WellDepth[kcal/mol]  44.44
WellDepth[kcal/mol]  2.31
End
      Rotor      Hindered      ! 63 cm^-1      CH3
      Group              22 23 24
      Axis              19 20
      Symmetry          3
      Potential[kcal/mol]      4
0      0.103333259 0.223148058 0.123061533
End
      Rotor      Hindered      ! 10 cm^-1
      Group              19 20 21 22 23 24
      Axis              4 18
      Symmetry          1
      Potential[kcal/mol]      8
0.01195343      0.2797124      0.631229467      0.187441507      0
0.321374644      0.77244548      0.210585943
End
Frequencies[1/cm]  63
                28.7912
                79.0441
                97.7220
176.6484      203.3793      316.3168
348.4021      371.6784      389.1046
477.7321      485.4667      496.9637
515.3030      619.9604      627.8965
657.2454      691.5528      746.3446
768.6028      768.8787      799.7490
813.3370      853.1219      892.6143
931.4543      939.8204      956.9292
969.1551      993.7361      1037.8501
1040.2588      1046.6855      1057.5648
1144.3211      1161.4569      1172.6711
1210.1482      1252.8749      1277.2623
1344.1359      1385.5919      1393.0761
1411.4232      1459.0165      1467.3266
1474.0957      1475.1044      1530.7447
1595.4413      1614.3671      1657.0523
2118.1022      3015.3446      3070.3195
3083.2119      3148.1046      3149.9389
3155.9823      3161.1578      3168.8979
3173.6564      3186.4070      3434.7944
ZeroEnergy[kcal/mol]  2.31
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts1-2-----
Barrier      ts1-2  i1  i2
RRHO
Geometry[angstrom]  24

```

```

C   -3.6991765103  0.5715589621 -0.0082453105
C   0.1412514365 -1.2106173568  0.0327111227
C   -3.5763759946 -0.8357747581  0.0464690616
C   1.2827136024 -0.4344546731 -0.0067634796
C   -0.0942592816  1.5692186668 -0.0754008448
C   1.141906261  0.9817961058 -0.061676544
C   -2.575384954  1.3628969559 -0.0481742656
C   -2.3345984626 -1.4245449156  0.0602129842
C   -1.2807581212  0.7870198245 -0.035349062
C   -1.1546949389 -0.6363933284  0.0199760934
C   2.6168229722 -1.0781892239  0.0083981313
C   3.7826247139 -0.4882426904 -0.0238812471
H   -4.6844319796  1.0239303845 -0.0185614809
H   0.230468771 -2.2923208175  0.0747818701
H   -4.4691669214 -1.4503635938  0.0776323695
H   -0.1838343731  2.6501202707 -0.1174460867
H   2.0367119703  1.5938408085 -0.0927604265
H   -2.6666824861  2.4434966891 -0.0901971912
H   -2.2404081653 -2.5048094314  0.102203717
H   2.5732668394 -2.1752784008  0.0520625286
C   5.0414404221  0.2282552977 -0.0618788086
H   5.1407854075  0.9053855994  0.7958748657
H   5.1270558111  0.8357976334 -0.9716494972
H   5.914361981 -0.4431220088 -0.0422314993
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  229.9263
WellDepth[kcal/mol]  5.28
WellDepth[kcal/mol]  3.21
End
Frequencies[1/cm]  65
32.4267          45.3432
123.3654         129.9946         182.4128
276.3873         298.6003         324.7371
387.8631         403.0819         484.6640
518.9512         524.5410         555.7427
633.5105         639.9821         720.2631
750.9756         780.1446         780.1914
804.5984         835.5812         855.5777
876.7152         914.5850         939.2407
962.3259         974.9320         977.5220
994.1034         996.9307        1025.9402
1042.5261        1142.9842        1171.5683
1175.9770        1188.0821        1234.6328
1272.1696        1281.4879        1289.9437
1387.6760        1394.0300        1405.0048
1410.2414        1450.2695        1469.4698
1471.9188        1498.1351        1542.8688
1608.7994        1640.5962        1665.5352
1808.6714        2945.0512        2974.1684
3003.2755        3037.8531        3151.1478
3155.2547        3156.6042        3161.4629

```

```

3173.7696          3175.1765          3186.8189
ZeroEnergy[kcal/mol] -36.84
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-3-----
Barrier      ts2-3  i2  i3
RRHO
Geometry[angstrom] 24
C -3.7629695558 0.6187902644 0.0901283413
C 0.0613021541 -1.1672522323 -0.2465481121
C -3.6387474128 -0.7844949302 0.0842648782
C 1.2475395941 -0.369187977 -0.306068572
C -0.1637565081 1.6365150515 -0.2621663749
C 1.0661523857 1.0740636388 -0.3582126774
C -2.631566612 1.4104581951 -0.0176304622
C -2.3994513246 -1.376313116 -0.0238572519
C -1.3531654281 0.8393343516 -0.1307505668
C -1.2178009487 -0.5909423866 -0.1307184082
H -4.7422058805 1.0755312048 0.1754992386
H 0.1580801056 -2.2477405926 -0.2657275746
H -4.5267343771 -1.4020330856 0.1651521412
H -0.2702168308 2.7166411924 -0.2914041657
H 1.9509012625 1.6933909769 -0.4601152407
H -2.7230668305 2.492224576 -0.0182171189
H -2.3082859116 -2.4577130919 -0.027692139
C 2.5879104849 -0.985082728 -0.5781508719
C 2.639688458 -0.9098194274 0.7033827115
C 3.162197569 -1.0948416378 2.0598288668
H 3.1218415515 -1.3280317191 -1.458820599
H 2.4790890913 -1.7095863024 2.6537527585
H 3.2664767087 -0.1342502979 2.5730375167
H 4.1433452553 -1.5875149266 2.0473526825
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 495.1615
WellDepth[kcal/mol] 25.79
WellDepth[kcal/mol] 3.5
End
Frequencies[1/cm] 65
62.2443          91.5754
118.2179         161.5623         194.5210
270.8300         277.1322         300.4171
397.2849         407.0803         439.4227
464.1436         506.0859         520.2349
615.7716         626.1579         692.0752
735.6551         738.5551         756.9831
767.0231         800.1802         808.1683
869.9224         875.5091         889.1462
941.2330         943.5352         975.3791
980.5673         1030.5817        1043.5005

```

1052.5966	1084.5417	1136.5193
1162.6746	1168.6093	1178.3825
1223.2672	1261.2727	1287.4782
1318.9034	1359.8637	1400.3080
1409.2167	1443.8233	1464.7616
1466.5469	1471.3205	1512.4906
1562.4004	1622.8429	1627.6005
1871.8071	2990.3910	3058.9271
3079.1189	3138.1998	3150.4539
3152.9858	3156.7598	3163.0449
3171.3112	3174.3565	3185.9312
ZeroEnergy[kcal/mol] -14.26		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
!-----bar_ts3-4-----		
Barrier ts3-4 i3 i4		
RRHO		
Geometry[angstrom] 24		
C	-3.588856	0.122578 0.121594
C	0.5109	-0.902898 -0.116362
C	-3.205125	-1.230563 0.033565
C	1.522477	0.104935 -0.158968
C	-0.230558	1.802808 0.074402
C	1.084787	1.484662 -0.015039
C	-2.622571	1.113757 0.131701
C	-1.874153	-1.575346 -0.045863
C	-1.255581	0.796286 0.05372
C	-0.857324	-0.580313 -0.041192
C	2.864984	-0.137972 -1.347655
C	2.980895	-0.250293 -0.071725
C	3.901439	-0.570084 1.053345
H	-4.638878	0.384176 0.183566
H	0.808722	-1.944424 -0.177585
H	-3.964958	-2.00443 0.028266
H	-0.532204	2.841617 0.166991
H	1.843119	2.260113 -0.003478
H	-2.914288	2.156993 0.202358
H	-1.582434	-2.618257 -0.115334
H	3.200947	-0.18694 -2.368721
H	3.523613	-1.425401 1.621847
H	3.965558	0.274568 1.74634
H	4.90293	-0.803355 0.6866
Core RigidRotor		
SymmetryFactor 0.5		
End		
Tunneling Eckart		
ImaginaryFrequency[1/cm] 570.0222		
WellDepth[kcal/mol] 3.44		
WellDepth[kcal/mol] 23.0		
End		
Frequencies[1/cm] 65		
68.3130	90.9103	

135.7836	175.1180	189.4649
229.6581	282.2002	360.5092
393.4619	437.0928	470.7090
483.3880	509.2137	525.1297
611.6183	625.9095	646.3562
673.2161	675.6279	742.8164
756.0611	766.8413	806.8120
810.8880	856.2090	871.9601
912.5533	942.3865	946.0790
976.6454	982.3229	1041.4592
1043.5102	1048.4261	1143.1021
1165.7297	1170.0055	1198.5001
1231.4236	1264.7386	1288.2376
1322.7751	1362.4314	1399.0796
1408.7208	1444.5854	1463.7789
1474.9741	1481.4892	1513.9820
1562.4192	1623.3206	1626.8263
1825.8167	3024.1267	3078.2003
3108.8651	3151.9224	3154.3890
3158.1467	3163.5234	3172.4994
3175.6066	3186.7827	3277.6845
ZeroEnergy[kcal/mol] -14.32		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
!-----bar_ts4-8-----		
Barrier ts4-8 i4 i8		
RRHO		
Geometry[angstrom] 24		
C	-3.5991862122	0.0838823616 -0.0039122946
C	0.538119891	-0.8206544558 0.0259658928
C	-3.1723207626	-1.2633334935 0.013741405
C	1.4866326755	0.1832019129 0.0187110137
C	-0.2971992837	1.8434256057 -0.0089367875
C	1.0351436248	1.5359567998 0.0008662729
C	-2.6755906493	1.1028045443 -0.0114376403
C	-1.8314229446	-1.5660343577 0.0235304556
C	-1.2869106653	0.8228115271 -0.0016979724
C	-0.8533876674	-0.5379379516 0.0161543919
C	3.8602772288	0.8290852736 0.0214032237
C	2.9516612048	-0.1147731752 0.0290153244
C	3.3778196213	-1.5803221062 0.0490953584
H	-4.6594589387	0.3102848513 -0.0115032775
H	0.8384409503	-1.861364111 0.0394844995
H	-3.9090002751	-2.0588508247 0.0195433399
H	-0.6164677883	2.880639283 -0.0224693057
H	1.7758669965	2.3275304058 -0.0048431655
H	-3.000916506	2.1380108047 -0.0249923855
H	-1.5032851361	-2.60040362 0.0370921427
H	4.5929647932	1.6013873145 0.015165185
H	2.9972475911	-2.1083938116 -0.8307764769
H	2.9888185212	-2.0865931635 0.9380497031
H	4.4640377308	-1.6606256136 0.0552370973

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Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 695.1996
WellDepth[kcal/mol] 3.39
WellDepth[kcal/mol] 4.32
End
Frequencies[1/cm] 65
35.6166          88.8854
169.7470         181.8903         228.3699
242.1694         323.1540         351.1277
397.1980         454.1500         462.7956
485.6657         520.7131         527.3926
559.1763         599.6794         631.8000
664.2612         677.1194         759.8259
782.1021         784.0398         833.9823
872.3881         879.8362         906.8406
952.8431         963.4863         978.1540
982.5105         995.5790        1033.5354
1042.9559        1076.0430        1147.9570
1173.7809        1178.6307        1200.6489
1235.0106        1278.8742        1292.3319
1372.8444        1392.9063        1397.2116
1411.1815        1466.7757        1486.0202
1488.8302        1498.7849        1539.8911
1608.4020        1640.8842        1642.7027
1667.4036        3022.4354        3077.3784
3125.4385        3155.5317        3157.3057
3160.9501        3173.9631        3178.6169
3183.7206        3187.4239        3433.6649
ZeroEnergy[kcal/mol] -33.93
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts8-5-----
Barrier      ts8-5  i8  i5
RRHO
Geometry[angstrom] 24
C -3.6229139835 0.1254589992 -0.1487551243
C 0.492534337 -0.8708180601 -0.1514305063
C -3.2260497326 -1.2325584397 -0.147919074
C 1.451112727 0.118177294 -0.1575335261
C -0.2880730604 1.81363935 -0.156478315
C 1.0429805797 1.478673951 -0.1586966369
C -2.6784136739 1.1227665965 -0.1504211046
C -1.8935617418 -1.5658281249 -0.1483257059
C -1.2935399736 0.812801459 -0.1506887401
C -0.8917634241 -0.5597901186 -0.1488017975
H -4.6780050917 0.3750496036 -0.1486756222
H 0.7938141988 -1.9135074658 -0.1594900417
H -3.9809711277 -2.0108113645 -0.1474588602
H -0.5874406141 2.8567209169 -0.1642129859

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H    1.8013978412  2.253377243 -0.1727249466
H    -2.9806231679  2.1650182298 -0.152171675
H    -1.5883234782 -2.6071290608 -0.149033932
C    3.5981658021 -0.3195703531 -1.2521282798
C    2.9149108669 -0.222765308 -0.1369733865
C    3.5372039084 -0.4305327376  1.2361094387
H    4.6135848062 -0.5348088167 -1.5530933383
H    3.0380186322 -1.2550941071  1.7552476449
H    3.4052238069  0.4660385189  1.8505151336
H    4.6031265631 -0.6539422049  1.1662243815
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  51.6384
WellDepth[kcal/mol]  2.93
WellDepth[kcal/mol]  1.8
End
Frequencies[1/cm]  65
78.2882          146.0952
177.5632          191.7488          197.8492
281.1523          359.1626          367.5052
416.7248          455.3583          486.7135
521.1060          552.4550          566.0342
628.0350          667.3857          676.6094
689.7832          759.6893          780.1439
785.3934          833.4025          847.7952
867.7927          875.5322          913.6508
956.2948          964.4081          977.9071
995.5809          996.9793          1030.1313
1041.4268         1080.7433          1152.6069
1170.6366         1178.3973          1207.4966
1239.8122         1278.2677          1289.4884
1371.8731         1392.8005          1395.2862
1399.7809         1463.8124          1477.8621
1481.0579         1499.5389          1539.2534
1606.2294         1640.5164          1669.2044
1681.0619         3017.2047          3071.9064
3108.4073         3156.2750          3158.9152
3160.7786         3163.5322          3174.5731
3180.9691         3187.4198          3226.3700
ZeroEnergy[kcal/mol] -35.32
ElectronicLevels[1/cm] 1
0  2
End
!-----
!-----bar_ts5-6-----
Barrier      ts5-6  i5  i6
RRHO
Geometry[angstrom]  24
C    -3.5868007287  0.1656043728  0.0328652642
C    0.4962542766 -0.8477742354  0.0885484196
C    -3.2180560395 -1.199705721  0.1329780007
C    1.4812807335  0.1100526309  0.0122036154

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C   -0.2284410914  1.7997883558 -0.1054918526
C   1.1114833455  1.4674920496 -0.0872638534
C   -2.6256160055  1.1419242913 -0.0446899109
C   -1.8966791662 -1.5645846663  0.15377219
C   -1.2435331204  0.8132022824 -0.0268967231
C   -0.8728317639 -0.579377391  0.0752319874
H   -4.6368347465  0.4350405238  0.0178748325
H   -3.9909944228 -1.9576770002  0.1933243775
H   -0.5263919417  2.8402826501 -0.1816778522
H   1.8663983841  2.2443435952 -0.1489419957
H   -2.9108135279  2.186400228 -0.1212499223
H   -1.6094241885 -2.6071199718  0.2301857504
H   1.3450155156 -1.9361773992  0.1654995985
C   2.7271350607 -1.842069564  0.151555867
C   2.8335815299 -0.5184033741  0.0523264933
C   4.0997433089  0.2848571204 -0.013886646
H   3.4452440758 -2.6486044844  0.2080917088
H   4.1424660291  0.8666267681 -0.9411254313
H   4.9818237331 -0.355336955  0.0290392019
H   4.1516227501  0.997099894  0.8168198804
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1985.2121
WellDepth[kcal/mol]  25.29
WellDepth[kcal/mol]  24.62
End
Frequencies[1/cm]  65
83.0835          114.5526
172.0516          179.5260          192.1321
232.2582          297.5574          397.9343
412.8113          453.0482          496.1916
503.6096          521.5282          563.0390
590.0119          647.6322          653.9617
668.4693          681.1581          758.0986
772.6170          794.1662          827.4686
873.1960          883.8911          941.0324
956.3463          968.5779          971.3883
996.0425          1012.6210          1028.2150
1035.7240          1052.2204          1141.3626
1150.4893          1166.2496          1179.4708
1235.2980          1262.1929          1315.1887
1364.0168          1373.0521          1381.0400
1408.6919          1459.2558          1480.5364
1482.5561          1485.5146          1540.0407
1586.8152          1617.4600          1647.4988
1664.4650          1748.3887          3016.1140
3063.2640          3111.2313          3155.2683
3158.4119          3166.4028          3175.3351
3178.4144          3189.1271          3217.9214
ZeroEnergy[kcal/mol]  -11.83
ElectronicLevels[1/cm]  1
0  2

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End
!-----
!-----bar_ts6-7-----
Barrier      ts6-7  i6  i7
RRHO
Geometry[angstrom]  24
C   -3.8818416507  0.5179733922  0.0923410731
C    0.0741927685 -0.9302104366  0.1943046931
C   -3.6585137401 -0.8453630549  0.3919063271
C    1.151769329  -0.1158667559 -0.0550590859
C   -0.3707225263  1.7239440514 -0.3883020509
C    0.917571213  1.2531200518 -0.3552836936
C   -2.822473284  1.3574020294 -0.1617008093
C   -2.3803696401 -1.3490019296  0.4330485359
C   -1.4891219579  0.8787371969 -0.1294961783
C   -1.266413474  -0.5094202077  0.1757941663
H   -4.8959384498  0.9002799798  0.063662942
H   -4.5038238843 -1.4947681526  0.5899382653
H   -0.5601300746  2.7677725647 -0.6165947774
H    1.7474658767  1.9217874169 -0.5568547851
H   -2.9962719413  2.4038156684 -0.3914889555
H   -2.2036174823 -2.3937801107  0.6622920259
C    3.6537604375 -0.3501508193 -0.1466545171
C    2.4288790482 -0.8501674395  0.0390090904
C    2.1182552688 -2.2868225905  0.386210609
H    3.8112829623  0.6937992234 -0.3949797362
H    4.5391913843 -0.9684291323 -0.0564018362
H    0.7927644011 -2.1048798059  0.421767446
H    2.4250169699 -2.6211281404  1.376749166
H    2.3219994461 -3.0254069989 -0.3883959146
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1823.649
WellDepth[kcal/mol]  15.79
WellDepth[kcal/mol]  39.94
End
Frequencies[1/cm]  65
47.7513          87.7916
173.7757         192.6830          230.9306
325.2686         348.6520          410.0579
418.5192         452.1716          500.9919
519.5031         521.4468          563.9605
588.0975         639.3369          652.3654
681.8384         728.0673          765.8900
789.1911         797.9509          831.1932
879.0055         894.9549          901.4062
929.8091         961.4452          962.0070
972.8280         997.2662         1033.2269
1040.9221        1041.7961          1132.1362
1147.4397        1170.0022          1179.7117
1234.5315        1238.8738          1263.3445
1306.4911        1362.7349          1365.9334

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1397.0405          1426.3130          1448.4897
1462.3296          1486.0932          1537.8860
1590.1835          1628.7694          1652.8016
1669.4116          1725.9372          3077.6711
3135.6816          3152.3194          3156.3528
3159.4385          3167.1740          3177.3461
3178.9267          3189.6819          3216.1468
ZeroEnergy[kcal/mol] -20.66
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts7-13-----
Barrier      ts7-13  i7  i13
RRHO
Geometry[angstrom] 24
C  3.496209878 -0.1220731838 0.2180543474
C  -0.5732033246 0.819472081 -0.451355826
C  3.1143552293 1.2088839637 -0.0409411006
C  -1.5893702111 -0.1932854716 -0.368837583
C  0.1674718034 -1.8545888379 0.0326831837
C  -1.14041576 -1.5677191837 -0.1634028552
C  2.5369156533 -1.1213979568 0.2482604109
C  1.7920545247 1.5261034674 -0.2599896875
C  1.1806194349 -0.8326065356 0.0295641358
C  0.7821098206 0.5237919145 -0.2264656626
H  4.5390546653 -0.3625249751 0.3892399904
H  -0.8685431355 1.838499976 -0.6767660329
H  3.8681409114 1.9881173278 -0.0675560166
H  0.4769941627 -2.8833864957 0.187842106
H  -1.8860439914 -2.3552210278 -0.1700134991
H  2.8289967749 -2.1489539283 0.4410674462
H  1.5012659596 2.5525149392 -0.4583282594
C  -3.7001633683 0.1627687834 -1.8896956486
C  -2.9762190131 0.0809796308 -0.7877320508
C  -3.0206917399 0.2259665457 0.6503183481
H  -3.2596673201 -0.0194816072 -2.8635047524
H  -4.7547550255 0.4143518004 -1.8493454461
H  -3.3401620241 -0.5953684095 1.2807291615
H  -2.9452599045 1.2054871832 1.1070932908
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 481.4375
WellDepth[kcal/mol] 36.15
WellDepth[kcal/mol] 1.25
End
Frequencies[1/cm] 65
70.6040          81.7781
165.3074          199.3003          216.1263
292.7356          358.3916          384.9391
432.5199          435.8733          471.9568
506.7616          517.7512          609.0075

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623.5365	668.2990	680.3744
719.9347	735.9969	751.3387
764.7324	789.0169	804.2074
836.4330	869.8436	887.4860
930.3889	936.4967	945.8746
960.9091	976.0436	982.2137
1023.0293	1043.8504	1065.8244
1144.2980	1167.6400	1169.9547
1187.4746	1219.6871	1261.6100
1290.3120	1325.5805	1358.7842
1409.8013	1422.7320	1441.9452
1457.9992	1467.0189	1511.3242
1561.3221	1622.1047	1631.6396
1808.6025	3124.1581	3129.3008
3153.4607	3155.6758	3158.9932
3167.0223	3173.2533	3177.2957
3187.4416	3215.9356	3224.7769
ZeroEnergy[kcal/mol] -24.45		
ElectronicLevels[1/cm] 1		
0 2		
End		
!-----		
!-----bar_ts13-14-----		
Barrier ts13-14 i13 i14		
RRHO		
Geometry[angstrom] 24		
C	3.4805307629	-0.1527829224 -0.1861075741
C	-0.6315102777	0.8184780489 0.0933407319
C	3.0692772748	1.1949528733 -0.2307313119
C	-1.6107947538	-0.2027369024 0.1792064448
C	0.1689594007	-1.8732369969 0.2109416319
C	-1.152893435	-1.5711252737 0.2853278084
C	2.5383477977	-1.1554857783 -0.0484209388
C	1.7347082737	1.5219682508 -0.1426634622
C	1.1665061997	-0.8560356645 0.0446072353
C	0.7407653961	0.5138233795 -0.0084559145
C	-3.3416272281	-0.0484791572 -2.298364245
C	-2.9982652784	-0.04662194 -1.0387060602
C	-3.0829969278	0.1274810344 0.3836803633
H	4.5335916481	-0.3995628148 -0.2564625067
H	-0.9461301792	1.8567989636 0.0750719871
H	3.8114378901	1.9787740558 -0.335969267
H	0.4927970828	-2.9063217581 0.2877933244
H	-1.890592686	-2.356776972 0.4104940596
H	2.8505152402	-2.1943804762 -0.0078603588
H	1.4225593593	2.5606619345 -0.1789643151
H	-2.6373521891	-0.3004198448 -3.0882558684
H	-4.3568615897	0.2007112584 -2.619098669
H	-3.6465657918	-0.6237365714 0.9395597868
H	-3.2862999894	1.1340782735 0.7547191179
Core RigidRotor		
SymmetryFactor 0.5		
End		
Tunneling Eckart		

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ImaginaryFrequency[1/cm]  552.2467
WellDepth[kcal/mol]  9.21
WellDepth[kcal/mol]  20.04
End
Frequencies[1/cm]  65
63.4556                72.2755
154.3139               183.2280                246.7529
265.8908               315.1035                391.7663
401.3315               424.1417                464.1634
500.8942               503.9604                521.3806
613.4106               627.9594                689.1816
739.7619               755.0382                768.6371
802.6995               806.8571                867.4681
872.1982               908.5553                921.7956
943.1635               946.2164                948.2678
970.4691               981.6406                1012.8384
1043.6707              1083.9274                1132.4137
1166.5901              1171.7804                1174.1159
1182.9455              1225.3112                1266.6996
1288.9568              1365.3991                1370.4587
1413.5830              1431.9182                1455.5328
1456.5815              1473.0919                1520.9153
1567.3872              1625.9140                1630.9200
1811.6093              3036.3845                3041.2117
3104.6345              3131.5910                3152.9021
3154.6817              3157.6731                3161.2967
3172.1744              3174.0049                3186.5421
ZeroEnergy[kcal/mol]  -16.49
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts14-15-----
Barrier      ts14-15  i14  i15
RRHO
Geometry[angstrom]  24
C   -3.6381931796  0.5687237009  0.438517266
C    0.1086092049 -1.2963855932 -0.2580781774
C   -3.4897495493 -0.8232137723  0.6383797838
C    1.1758806348 -0.541035156 -0.6785407351
C   -0.1821778085  1.4942891566 -0.6606334797
C    0.9947235226  0.8437696795 -0.8682791983
C   -2.5711305541  1.3248510116  0.0179777706
C   -2.2781904782 -1.430313433  0.413820573
C   -1.3055008572  0.7303245679 -0.2234488197
C   -1.1526135048 -0.6820794744 -0.021262363
H   -4.5992462097  1.0371571451  0.6189135446
H    0.2064613301 -2.3670039374 -0.099916244
H   -4.3384995487 -1.4105221848  0.9704436025
H   -0.2926050192  2.5630899782 -0.8150634318
H    2.2830883593  1.1325774002 -1.2683276063
H   -2.6824793217  2.3931825947 -0.1361212454
H   -2.1649023472 -2.4985935589  0.5673835323
C    2.5957591964 -0.9871643407 -0.9875072348

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C    4.5307710461  0.5799157753 -1.783919393
C    3.3099192901  0.2734267616 -1.3991753297
H    3.0719098176 -1.4451841582 -0.1125049994
H    2.6160803878 -1.7345750636 -1.7894390802
H    5.3157620643 -0.1730881796 -1.8673473504
H    4.8128075268  1.5974880821 -2.0361883757
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1834.8619
WellDepth[kcal/mol]  24.36
WellDepth[kcal/mol]  19.84
End
Frequencies[1/cm]  65
43.4119          113.4332
173.9459          175.4407          258.3364
264.8237          312.4579          373.2318
391.9182          432.6302          480.7253
509.9273          557.7966          562.8356
590.0260          643.6265          648.3027
751.9746          754.8638          776.3413
778.0881          854.5739          871.1259
885.2161          902.1320          909.4661
912.1373          955.0632          956.0757
966.7788          994.4498          1042.4529
1067.0546          1089.7318          1143.1655
1168.7106          1171.6662          1174.9726
1217.6649          1243.0028          1257.6968
1277.2043          1348.2516          1388.2974
1402.1123          1424.6846          1445.3244
1461.9967          1476.0287          1533.8072
1609.1104          1631.9751          1658.1793
1726.1091          1735.4890          3012.2901
3039.3973          3074.8563          3146.4066
3156.3643          3157.6699          3162.2286
3169.0387          3174.4428          3187.1480
ZeroEnergy[kcal/mol]  -12.17
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts14-16-----
Barrier      ts14-16  i14  i16
RRHO
Geometry[angstrom]  24
C    -3.6459303061  0.3230051641  0.1580253701
C    0.3754595695 -0.9238724811 -0.087141799
C    -3.3514322537 -1.05987104  0.1904304491
C    1.401513926 -0.0247031358 -0.1971672571
C    -0.2089165568  1.7683341399 -0.1494275888
C    1.1013245341  1.3585911173 -0.2291765041
C    -2.634125522  1.246392728  0.0481034817
C    -2.051229674 -1.4975717583  0.1125113166

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C   -1.2783993394  0.8368775049 -0.034972831
C   -0.9838222409 -0.5705900573 -0.0016134867
H   -4.6770442965  0.6521617996  0.2205194984
H    1.1355589518 -2.0763165895 -0.0977127075
H   -4.1603596966 -1.7765889647  0.2774726712
H   -0.4485398853  2.826419091 -0.1731780575
H    1.898583925  2.0903439909 -0.3159574306
H   -2.8610115827  2.3075144725  0.0233028168
H   -1.8208692868 -2.5566997036  0.1369804433
C    2.7694145679 -0.6778641634 -0.2716356019
C    3.1927995221 -3.2566515417 -0.2017457813
C    2.4760760041 -2.1529356478 -0.1925955825
H    3.2891449887 -0.4225630412 -1.2033698168
H    3.4174687349 -0.3540068633  0.5521164173
H    4.2806245565 -3.2366277474 -0.2819046249
H    2.7346453601 -4.2383002731 -0.1299433947
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  1836.7489
WellDepth[kcal/mol]  23.83
WellDepth[kcal/mol]  18.79
End
Frequencies[1/cm]  65
51.7861           111.7265
157.2918          169.1925          250.8709
262.2797          313.8908          387.6156
412.2045          471.5348          495.4771
509.5303          514.9701          554.1863
563.4579          641.5179          651.7169
736.5858          753.1768          778.7085
797.7136          820.7294          877.0657
895.1438          910.7621          936.1128
950.7713          962.5021          972.3043
973.2643          996.2412          1040.5871
1040.7551          1095.4464          1140.9118
1164.1746          1167.6574          1172.8969
1202.8400          1234.6950          1259.1305
1292.4016          1365.0604          1371.5734
1390.0518          1424.4849          1458.5661
1463.3997          1489.9967          1538.1530
1589.6900          1633.7118          1661.5994
1726.4216          1740.0278          3006.4598
3031.8991          3075.0358          3152.3173
3156.4389          3166.1261          3168.6207
3171.7061          3178.1978          3188.9897
ZeroEnergy[kcal/mol]  -12.7
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts15-17-----
Barrier      ts15-17  i15  i17

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RRHO
Geometry[angstrom] 24
C -0.1009863622 -0.6413943597 0.0669605441
C -1.5129241897 -1.2262975441 0.1267092102
C -2.4155360612 -0.1221574557 -0.3574847198
C -2.2634148373 1.106196934 0.2133992338
C -0.0087189753 0.7610705448 0.0066957474
C 1.1526743152 1.4603441893 -0.05428818
C 2.3808112705 0.7291264758 -0.0653410143
C 2.3327539715 -0.7020911808 -0.0041662042
C 1.0729504015 -1.3597941914 0.0624784523
H -1.597819414 -2.130975847 -0.4792668577
H -1.7474871924 -1.5108562502 1.1611680519
H -2.8890653677 -0.2191664988 -1.3289162558
H -1.9712464 1.2105556944 1.2527646311
H -2.6893116855 1.9938916416 -0.2421935133
H 1.1796229439 2.5450874774 -0.0982697091
H 1.0550571205 -2.445973121 0.1059018237
C 4.8071527991 0.6405354966 -0.1445388556
C 4.7625885319 -0.7711624461 -0.0837349118
C 3.643276487 1.371444268 -0.1363225644
C 3.5552173234 -1.4235760108 -0.0160450132
H 5.7654486779 1.1451482157 -0.1978387542
H 5.6870300693 -1.3376775139 -0.0910316061
H 3.6753796694 2.4551251874 -0.1832530562
H 3.5208389041 -2.5073267054 0.0297765213
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 417.0066
WellDepth[kcal/mol] 10.83
WellDepth[kcal/mol] 44.17
End
Frequencies[1/cm] 65
69.9086 114.4662
191.6696 233.6131 254.5551
297.7749 393.8645 397.4929
421.2474 479.6463 489.8505
524.6141 555.5788 623.1846
635.0302 681.5692 723.2970
753.9803 771.6017 775.2417
848.9654 853.7004 867.7043
894.4591 903.4378 921.3709
940.6993 954.7401 960.4611
964.4494 992.7961 1042.3821
1081.0420 1138.4413 1167.7780
1169.5527 1203.9975 1215.6754
1237.2066 1266.1656 1274.8515
1289.2590 1344.2389 1387.4071
1398.8457 1421.1839 1439.0030
1472.6548 1480.2958 1531.5712
1564.2559 1604.6850 1622.7128
1655.8238 2999.2021 3078.7614

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3126.1363          3139.5968          3149.9249
3155.8352          3160.9781          3161.3104
3173.5632          3186.4111          3207.2985
ZeroEnergy[kcal/mol] -21.18
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts16-18-----
Barrier      ts16-18  i16  i18
RRHO
Geometry[angstrom] 24
C  -0.1432039942 -0.5803318662 0.0369707311
C  -1.5258759072 -1.2307635757 0.0427413195
C  -2.4726788448 -0.1294462158 -0.3552930455
C  -2.342219832  1.0723776643 0.2771326436
C  -0.0912721248 0.7834708035 0.0173503292
C  1.0867804783  1.5468484064 0.0240267514
C  2.3245309056 0.8117621713 0.0401411363
C  2.2806716151 -0.6088887133 0.056613786
C  1.0865904957 -1.290353917 0.0572334104
H  -1.5710322967 -2.0802564178 -0.6437429668
H  -1.7477003216 -1.6223971428 1.0450277988
H  -2.9679621436 -0.1875103007 -1.3189181701
H  -2.0380610529 1.1320414566 1.3162709889
H  -2.8073067917 1.9668516734 -0.1241473645
H  3.2178408947 -1.1556065919 0.0690265699
H  1.0804011567 -2.3764876717 0.0724394522
C  2.3283340649 3.631668952 0.0140752384
C  3.5466079174 2.9127852157 0.0280086362
C  1.1268429987 2.9656000087 0.0112082135
C  3.5429412978 1.5387163977 0.0397604594
H  2.347459705 4.7157533709 0.004274987
H  4.4866416842 3.4530724896 0.0290494597
H  0.1898455737 3.5104110502 -0.0032974899
H  4.4786345217 0.9885627527 0.0505591255
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 424.2524
WellDepth[kcal/mol] 10.17
WellDepth[kcal/mol] 44.68
End
Frequencies[1/cm] 65
81.8095          111.2943
185.4572          206.1254          243.1694
290.5527          408.2988          414.5569
448.0430          493.3601          501.4352
516.3327          531.8734          606.8830
637.5621          654.9188          739.3103
753.0058          765.1792          776.1009
817.2667          874.8398          876.1157
911.7520          925.5851          943.5622

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956.1049	958.5528	967.1779
969.3345	995.0029	1039.4755
1083.8976	1136.0867	1166.2766
1170.2372	1199.0524	1202.9898
1234.3784	1259.6136	1275.0374
1294.2257	1360.9109	1364.6547
1388.2157	1421.9694	1453.4587
1479.4952	1490.1698	1528.0272
1564.6986	1583.7174	1635.9549
1661.1497	2994.0570	3067.2195
3126.7929	3146.4089	3155.1423
3161.4757	3165.5927	3170.3377
3178.7808	3188.9098	3207.0571

ZeroEnergy[kcal/mol] -21.32
 ElectronicLevels[1/cm] 1
 0 2
 End
 !-----
 !-----bar_ts2-9-----
 Barrier ts2-9 i2 i9
 RRHO
 Geometry[angstrom] 24
 C -3.670911 0.563115 -0.055287
 C 0.172469 -1.207409 0.028436
 C -3.542428 -0.844515 -0.090372
 C 1.32134 -0.429923 0.077482
 C -0.071491 1.570716 0.103473
 C 1.167602 0.990582 0.124772
 C -2.550161 1.358218 0.006523
 C -2.299602 -1.430047 -0.062941
 C -1.255085 0.786221 0.035457
 C -1.12213 -0.637798 -0.000211
 C 2.630173 -1.079581 0.099849
 C 4.514936 0.664363 -0.282089
 C 3.832494 -0.479426 0.200913
 H -4.657241 1.012598 -0.077245
 H 0.263411 -2.289273 0.005079
 H -4.43239 -1.462099 -0.138919
 H -0.165013 2.65142 0.141785
 H 2.047898 1.617492 0.190634
 H -2.645441 2.438968 0.034107
 H -2.201707 -2.510448 -0.089445
 H 2.602942 -2.16698 0.122732
 H 5.355744 1.05674 0.281791
 H 4.136162 1.280112 -1.1017
 H 4.932392 -0.57563 -0.484838
 Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 1840.5094
 WellDepth[kcal/mol] 42.2
 WellDepth[kcal/mol] 67.84
 End

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Frequencies[1/cm]  65
44.8884           111.0161
123.5777           182.7056           224.6447
246.0666           356.9728           386.0985
394.5739           419.0170           436.2324
485.3116           525.4288           548.8213
614.9455           643.7327           661.0778
756.9064           762.4833           780.7614
781.6549           829.8254           837.5241
872.5340           877.8592           893.1396
908.0433           960.9959           963.1615
977.7526           992.8993          1033.0360
1041.6315          1047.5297          1130.4938
1147.9022          1174.0803          1181.2397
1197.2480          1242.6988          1285.0576
1289.5353          1327.3065          1391.8523
1398.0698          1411.1548          1457.9116
1470.9604          1498.4362          1539.7948
1592.2819          1602.0953          1637.3727
1663.0839          2179.2987          3034.8536
3120.0971          3153.4469          3156.1211
3158.6145          3161.8742          3171.5300
3173.9154          3186.9488          3193.0413
ZeroEnergy[kcal/mol]  2.15
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts2-12-----
Barrier      ts2-12  i2  i12
RRHO
Geometry[angstrom]  24
C   -3.7727890263  0.2863751064 -0.2136799032
C    0.3336324293 -0.7156336317  0.0321040207
C   -3.3335043518 -0.9973423667 -0.6094816565
C    1.2626176909  0.2124099837  0.4961132915
C   -0.5247868595  1.8319269816  0.8202901151
C    0.799667178  1.5048519581  0.9021841118
C   -2.867068717  1.2121330215  0.2529721114
C   -2.0029240536 -1.332697886  -0.5317519429
C   -1.4902022405  0.8999692345  0.3444887581
C   -1.0421561725 -0.4004880431 -0.0547093461
C    2.6433183229 -0.1334831167  0.650630221
C    3.8723105991 -0.3911901764  0.353809568
C    4.9019770383 -0.3701022832 -0.7246392218
H   -4.8250348671  0.5385701437 -0.27969995
H    0.6685998008 -1.7013982441 -0.2710215211
H   -4.053973872  -1.7200153239 -0.9763335487
H   -0.858124332  2.820345851  1.1198967706
H    1.5212559947  2.2248087565  1.2706196442
H   -3.2002604955  2.1992094138  0.5572894806
H   -1.6673931483 -2.3188809422 -0.8355715168
H    3.4271098279 -0.4468974138  1.598360145
H    4.4527746578 -0.057731903  -1.6769636705

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H    5.3497737299 -1.358364457 -0.8540998213
H    5.7064378665  0.3263253369 -0.4753191393
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  2063.8455
WellDepth[kcal/mol]  45.52
WellDepth[kcal/mol]  51.41
End
Frequencies[1/cm]  65
38.3242          56.5027
106.5917         143.9561          179.3810
210.7578         234.0482          277.6966
359.0963         381.0999          396.6021
436.9417         478.7727          515.3278
541.5490         551.0481          621.7835
650.9750         659.2419          754.2864
775.9563         776.6025          824.8125
848.5920         861.7357          892.1744
933.2267         956.2777          974.3634
975.2726         989.6517        1026.3258
1029.9818        1042.2281        1139.2416
1170.5084        1175.2967        1181.7476
1229.0756        1273.5844        1287.6262
1356.9008        1383.8837        1388.1801
1403.5557        1460.6388        1465.8389
1475.4320        1487.9764        1530.7444
1588.1034        1629.3027        1653.1133
1967.3961        2298.2520        2987.1793
3073.4829        3094.9856        3155.6344
3158.7775        3161.2537        3171.9116
3174.4061        3183.1341        3187.2601
ZeroEnergy[kcal/mol]  5.47
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts9-10-----
Barrier      ts9-10  i9  i10
RRHO
Geometry[angstrom]  24
C    0.0643016429 -0.4228854266 -0.1237875015
C    1.3897298712 -0.8910148288 -0.2028115431
C    2.582806753 -0.0456520088 -0.4043629242
C    3.3507965018  0.444956116  0.5667686131
C   -0.2534541888  0.9831233054 -0.1767453424
C   -1.5412375719  1.420319688 -0.1021463528
C   -2.6347284779  0.5108781109  0.0348348289
C   -2.3489414783 -0.8926718316  0.0936355221
C   -1.0104680552 -1.3254259313  0.0121772803
H    1.5448951689 -1.9671888212 -0.1738278164
H    2.8588381221  0.1674953458 -1.4400551945
H    3.1290161417  0.2642375623  1.6134684153

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H   4.2278332655 1.0429326546 0.3436366448
H   0.5593168297 1.6930348805 -0.2715068389
H  -1.7567356226 2.4833585 -0.1447654678
H  -0.8011555407 -2.3899006145 0.0553860384
C  -3.9752839429 0.9432762239 0.1148327007
C  -5.0061510846 0.0360926901 0.2478909686
C  -4.7298087586 -1.3474923105 0.3063337141
C  -3.4339968816 -1.8013990241 0.23118785
H  -4.1859588077 2.0069435583 0.0697634652
H  -6.0315449284 0.3825866228 0.3080214394
H  -5.5464570533 -2.0530680102 0.4109277826
H  -3.2218749043 -2.8646144509 0.2759017181
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 176.0874
WellDepth[kcal/mol] 10.16
WellDepth[kcal/mol] 6.47
End
Frequencies[1/cm] 65
58.9884          118.1762
143.3594          186.5372          265.7495
284.2813          380.4698          392.5955
449.1184          474.9843          493.4555
516.1377          522.6251          617.3919
630.5494          660.8328          696.4010
756.6212          772.2065          772.8247
795.0997          827.3279          857.3025
885.7284          886.2816          951.1393
957.6710          959.9595          985.7775
989.4040          991.4129          1014.6431
1042.4218          1097.0442          1145.4287
1165.3729          1172.6588          1202.2104
1235.9989          1275.2230          1290.7650
1315.1615          1339.4717          1380.6597
1403.6935          1420.7562          1452.0834
1471.4569          1482.3140          1529.4492
1573.0427          1622.1227          1640.3165
1685.8856          3066.8506          3127.4896
3131.0439          3155.6143          3157.5864
3158.6182          3162.7295          3174.8984
3188.0176          3188.9740          3212.8347
ZeroEnergy[kcal/mol] -55.53
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts10-11-----
Barrier      ts10-11  i10  i11
RRHO
Geometry[angstrom] 24
C  -3.3739532523 -0.704195826 0.2102618768
C  0.3321079162 1.3453331891 -0.1274975412

```

```

C   -3.3244095633  0.6919479127  0.3921330466
C   1.4797690611  0.6620262567 -0.4065720699
C   0.2077095433 -1.4411678799 -0.5677662002
C   1.4417111064 -0.7754455026 -0.6686786223
C   -2.2266103601 -1.4074286318 -0.0859313278
C   -2.1221946551  1.3630651738  0.2714399208
C   -0.9752521461 -0.7497610903 -0.2101411625
C   -0.9307625381  0.6745010228 -0.0319171198
C   2.8471559923  1.1543615733 -0.2297821526
C   3.0331010124 -1.0420290375  0.7008520554
C   3.6638662686  0.2283695206  0.3088550897
H   -4.3199098866 -1.2257236294  0.3051636068
H   0.3737292178  2.4053531832  0.1043445728
H   -4.2312230356  1.2384837711  0.6247705428
H   0.1403130886 -2.4928423342 -0.8258961787
H   2.1584629406 -1.1621295561 -1.3868609753
H   -2.2655680998 -2.4826500851 -0.2273757269
H   -2.0830576113  2.4388723645  0.4097172439
H   3.1452496515  2.1689305874 -0.4672785354
H   3.5757319853 -1.9712426586  0.5439125781
H   2.4233495128 -1.0356124382  1.60002074
H   4.7296158513  0.3954821143  0.444608339
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  621.5095
WellDepth[kcal/mol]  29.46
WellDepth[kcal/mol]  23.64
End
Frequencies[1/cm]  65
87.0073           120.4135
193.8175          237.5361          286.0566
373.3478          390.9271          415.7222
457.4084          477.5963          526.8128
550.8634          597.2274          625.7282
645.7777          697.3885          731.8933
746.7738          758.7195          767.0185
793.4221          815.4478          818.7634
867.6585          890.9094          907.7001
942.8676          946.9894          952.1300
978.6937          983.1936          1018.6405
1045.8767         1071.5331          1131.4842
1146.3334         1160.5607          1173.5546
1182.2031         1223.0369          1264.8283
1286.9847         1340.4356          1367.7386
1377.3147         1409.3005          1447.9204
1463.4458         1481.7870          1515.1094
1571.4150         1601.4991          1628.7793
1633.2321         3098.7111          3127.7735
3134.1847         3153.4812          3155.7699
3159.5911         3164.9142          3173.2998
3179.1937         3186.5178          3187.2287
ZeroEnergy[kcal/mol]  -32.54

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ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts11-p1-----
Barrier      ts11-p1  i11  p1
RRHO
Geometry[angstrom] 24
C   -3.4161438987 -0.7006126056 0.0442542038
C    0.2505748051 1.4366481775 0.0112789432
C   -3.4182470513 0.7118164046 0.002333923
C    1.4318570431 0.7422279309 0.0134792004
C    0.2518916741 -1.4022025397 0.0602640149
C    1.4405948539 -0.7013218814 -0.0420101523
C   -2.2266650169 -1.3890986047 0.0625873534
C   -2.2315107672 1.407009672 -0.0173981907
C   -0.9831193735 -0.7052893886 0.0385278868
C   -0.9855906829 0.7313394804 0.0002815872
C    2.8189811523 1.1890458287 0.0952635723
C    2.8717797653 -1.1704433589 0.1746376969
C    3.6419402452 0.1291895689 0.1758934097
H   -4.3569356707 -1.2391150222 0.0603955891
H    0.2388938465 2.5216348836 0.036533428
H   -4.3611342106 1.2468451352 -0.012689904
H    0.2465869783 -2.4867971317 0.1031272278
H    1.5799159402 -0.7667877778 -1.908343318
H   -2.2225555069 -2.4738791022 0.0918442281
H   -2.2342754444 2.4917755546 -0.0462141572
H    3.1224621046 2.2282584996 0.0988003843
H    3.2233463442 -1.8717554671 -0.5870037976
H    2.9650742172 -1.6799011958 1.1431078996
H    4.720848653 0.1725469397 0.2497909715
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 781.0149
WellDepth[kcal/mol] 25.88
WellDepth[kcal/mol] 6.21
End
Frequencies[1/cm] 65
102.2842          131.8339
249.2988          262.0147          280.6743
382.1412          390.5720          413.0913
424.7886          470.9704          482.5557
528.8816          558.2109          578.6936
627.6745          694.4021          732.3464
745.8256          748.1660          765.1017
779.6125          805.6296          853.4539
856.6266          884.5213          902.9943
913.6281          954.6612          957.2314
963.2458          971.9009          991.9228
1043.3690         1074.9416         1122.2664
1160.3921         1167.4599         1172.5039

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1179.3466	1241.3644	1249.0100
1270.9740	1282.9909	1348.9356
1372.5964	1383.9238	1427.8524
1444.8274	1459.0676	1484.4678
1531.9691	1601.2034	1617.7054
1649.5553	1653.7774	3010.0272
3065.3924	3156.6358	3160.1185
3161.4879	3164.2620	3175.0274
3188.0466	3190.5188	3212.6235

ZeroEnergy[kcal/mol] -30.3
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts17-p1-----
Barrier ts17-p1 i17 p1
RRHO
Geometry[angstrom] 24
C -3.4369578331 0.699696125 -0.0486182351
C 0.2402614229 -1.4032714515 0.11476639
C -3.431640392 -0.7118613356 0.0271930958
C 1.4145539726 -0.6917912282 0.0959723728
C 0.2316509305 1.4259228209 -0.0349559104
C 1.4093791552 0.7342530315 0.0219705851
C -2.2518320656 1.3955101098 -0.0694397383
C -2.2423500575 -1.3975733853 0.080737623
C -1.0054560598 0.7209352702 -0.0162292488
C -0.9992869648 -0.7119312129 0.0614334405
C 2.8159995184 -1.1352648554 0.140940076
C 2.8400136329 1.2280571847 0.033322442
C 3.6314907978 -0.0481038022 0.1639045731
H -4.3808073277 1.2315641793 -0.0906769188
H 0.2411595473 -2.4873322443 0.1651261945
H -4.3716991825 -1.2519015628 0.0425885025
H 0.2164642023 2.5103606366 -0.0899849907
H -2.2548793033 2.4792355334 -0.1276599684
H -2.2373209736 -2.4812230356 0.1383096626
H 3.1242375647 -2.154704391 0.3305457
H 3.0377996964 -1.7191708869 -1.7517158024
H 3.0381401978 1.9179435674 0.8631555812
H 3.0967958085 1.7714954761 -0.8861628943
H 4.7109197126 -0.0740495431 0.2313574681
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 622.3339
WellDepth[kcal/mol] 33.17
WellDepth[kcal/mol] 4.33
End
Frequencies[1/cm] 65

101.0191	130.6583	
238.5014	260.5263	267.6723
284.0391	339.3300	400.4518

407.3612	419.4070	464.9340
487.9126	565.1893	578.5002
628.8708	703.1001	730.0184
732.6100	750.6896	761.8662
782.9217	804.6804	856.1237
859.4452	888.6001	904.6448
913.7844	953.8285	957.7055
965.4928	978.3205	992.9148
1043.3144	1073.1750	1114.9212
1152.3385	1169.4191	1173.8758
1179.5237	1244.0658	1250.0400
1267.9018	1282.4122	1346.3839
1371.7265	1388.7757	1431.1763
1443.3502	1471.5625	1485.1794
1533.1696	1555.5160	1620.3513
1654.1445	1678.4667	3004.3221
3028.6417	3154.5124	3156.7573
3160.4458	3164.8346	3174.1907
3187.2735	3197.5379	3216.2095

ZeroEnergy[kcal/mol] -32.18

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts18-p2-----

Barrier ts18-p2 i18 p2

RRHO

Geometry[angstrom] 24

```

C 3.3467707902 -0.1785645617 0.0283128244
C -0.8816778736 -0.4308823346 0.0772987843
C 2.7266341807 -1.4474179326 0.0880953707
C -1.6321784739 0.736130503 0.0179818621
C 0.3623896443 2.0670396569 -0.0625745804
C -1.0124464836 1.9960327066 -0.0543042517
C 2.5830000004 0.962201947 -0.0181305528
C 1.356140247 -1.5512903354 0.1040311628
C 1.1651668353 0.895098189 -0.005705428
C 0.5386850548 -0.3934255842 0.0615287619
C -3.1000284955 0.3871655742 0.0465062112
C -1.8059199662 -1.5749763316 0.1380467099
C -3.084326966 -1.1118664159 0.1685428543
H 4.4287631125 -0.1100948359 0.0169816551
H 3.3385110245 -2.3419746037 0.1195807407
H 0.8580145605 3.0307197271 -0.1141791825
H -1.60855089 2.9014505345 -0.0999804279
H 3.0574186703 1.9369425639 -0.0676418429
H 0.8891385175 -2.5285052108 0.1443867391
H -3.6267749799 0.8603741702 0.8852338262
H -3.6182466881 0.7157557167 -0.8650690172
H -1.676550226 -2.21782164 -1.7679862611
H -1.511687486 -2.5982159243 0.3245781513
H -3.9761071127 -1.7189895784 0.2426998906

```

Core RigidRotor

SymmetryFactor 0.5

```

End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  584.6788
WellDepth[kcal/mol]  33.76
WellDepth[kcal/mol]  3.95
End
Frequencies[1/cm]  65
112.4164          129.4980
220.0739          236.9861          257.0120
277.0483          325.2868          411.4650
432.8203          459.6675          465.0089
506.9468          520.0546          573.4841
612.4456          680.1152          681.7616
715.6635          749.0727          752.7342
795.8643          818.3622          838.5234
878.6929          881.4388          931.3389
955.4615          958.3760          964.0995
968.9134          970.9573          994.0877
1044.3388         1071.3674          1118.2353
1141.5589         1167.5365          1178.7593
1190.5671         1216.4532          1236.6844
1283.2221         1295.0235          1351.1644
1378.1271         1391.3406          1426.5056
1430.1058         1469.1431          1486.5262
1534.1385         1559.4398          1606.6074
1630.8603         1665.1349          3005.3037
3029.5644         3156.7955          3158.7443
3166.7688         3175.6821          3179.5194
3189.3967         3204.2806          3222.7236
ZeroEnergy[kcal/mol]  -32.24
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts18-p3-----
Barrier      ts18-p3  i18  p3
RRHO
Geometry[angstrom]  24
C   3.349603819 -0.1594102526 0.0679420742
C   -0.8707816038 -0.4482471378 -0.0565759073
C   2.7378703675 -1.4343031043 0.0898152056
C   -1.6309329152 0.7114966643 -0.1145524203
C   0.3505332656 2.0645921519 -0.0952555357
C   -1.0201847235 1.9847794732 -0.1326320294
C   2.5777738292 0.9755630688 0.0073462511
C   1.3695355147 -1.550060269 0.050393885
C   1.1617005376 0.8976080754 -0.0339763704
C   0.5420048961 -0.3974444147 -0.0121681545
C   -3.0553133895 0.3404122391 -0.1384823921
C   -1.793557454 -1.643687926 -0.0524545841
C   -3.158287826 -1.0144518751 -0.1519753011
H   4.4305061182 -0.0821729935 0.0994283084
H   3.3560972073 -2.323824692 0.1382419823
H   0.8405272018 3.0325394855 -0.1097156133

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H   -1.6254114514  2.8836673056 -0.172484604
H    3.0453978028  1.9547221748 -0.0091659716
H    0.9082011463 -2.5312612362  0.0680849631
H   -3.5279554691  0.7342791839  1.777385027
H   -3.8647175197  1.0371023739 -0.3106965168
H   -1.6010891699 -2.3276028261 -0.8890391808
H   -1.6917225942 -2.2430939383  0.8628032418
H   -4.0776085899 -1.5820215306 -0.1978263569
Core  RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  589.455
WellDepth[kcal/mol]  33.74
WellDepth[kcal/mol]  4.06
End
Frequencies[1/cm]  65
109.5879          136.2343
229.1242          235.9090          245.0631
272.7382          327.4880          415.3083
433.3986          456.8034          466.0924
520.4280          520.7401          559.3633
616.6651          680.9692          682.6230
714.6209          751.3308          759.5856
787.1069          827.9317          837.1055
870.3633          873.6078          934.1078
956.0166          958.5071          969.0396
972.1533          981.2748          993.1017
1044.0631         1059.1819         1110.1577
1143.6812         1167.3835         1179.3712
1185.0134         1232.9051         1241.4102
1266.3958         1288.5925         1361.1555
1377.9802         1397.9462         1415.9582
1432.6389         1467.9509         1488.4644
1535.2150         1561.8297         1611.9057
1630.6281         1663.3817         3004.8694
3029.4418         3157.2792         3160.8015
3164.7244         3177.0407         3179.4833
3188.0262         3199.0570         3219.6524
ZeroEnergy[kcal/mol]  -32.27
ElectronicLevels[1/cm]  1
0  2
End
!-----
!-----bar_ts12-p4-----
Barrier      ts12-p4  i12  p4
RRHO
Geometry[angstrom]  24
C   3.8494578241  0.0133955988 -0.0961380097
C  -0.2911225313 -0.8265479342  0.0948842842
C   3.4021715112 -1.3283169831 -0.0691067797
C  -1.2174944552  0.204481585  0.1310021555
C   0.5859118177  1.8319946724  0.0403996317
C  -0.7531367127  1.5549402461  0.102302238

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C   2.9443252415  1.0471454419 -0.0607866765
C   2.059655448  -1.6108033656 -0.0071516199
C   1.5517938601  0.7908698527  0.0032861888
C   1.0977969537 -0.5660036235  0.0310897513
C  -2.6119376481 -0.0645497721  0.1980216906
C  -3.8064177326 -0.2793046881  0.1818474905
C  -5.2210016373 -0.5379921904  0.4408899057
H   4.9120872249  0.2224954824 -0.1453491184
H  -0.635976408 -1.8540768318  0.1148228041
H   4.1263542287 -2.1345973167 -0.097955158
H   0.926694903  2.8618680895  0.0177568432
H  -1.4820615265  2.3556052228  0.1287871922
H   3.2860561589  2.0767512387 -0.0819579015
H   1.7147407221 -2.6392681578  0.0131765332
H  -3.9955378372 -0.3148420439 -1.924446239
H  -5.4091081128 -0.5775786362  1.5181810984
H  -5.5337759884 -1.4895547788  0.003768454
H  -5.8492683039  0.2471568919  0.0127612413
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  425.5057
WellDepth[kcal/mol]  39.64
WellDepth[kcal/mol]  3.32
End
Frequencies[1/cm]  65
53.4538           62.5422
74.9951           136.8194           165.3837
183.0263          279.2070           305.6283
328.0119          373.6550           391.5432
402.1043          466.4501           485.3588
515.7630          557.2344           558.8004
617.5982          659.0138           661.7259
760.7467          779.0749           781.0812
833.6406          858.2031           875.6439
914.2711          951.5970           966.1441
981.2822          998.0836          1011.2170
1042.2855          1045.2865          1061.1751
1151.9282          1173.3863          1178.4243
1211.2272          1249.5762          1287.5086
1298.8388          1371.2273          1395.5124
1403.9579          1414.9346          1464.3868
1476.3920          1480.5800          1500.7272
1536.6110          1601.4894          1639.2873
1664.2171          2277.5550          3026.1221
3085.0693          3092.5693          3158.8822
3162.8109          3165.2170          3176.4407
3180.0431          3189.1717          3193.7348
ZeroEnergy[kcal/mol] -6.3
ElectronicLevels[1/cm] 1
0 2
End
!-----

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!-----bar_ts10-p5-----
Barrier      ts10-p5  i10  p5
RRHO
Geometry[angstrom]  24
C   3.7176063655 0.4397991611 -0.2198045521
C   -0.1810126658 -1.1477607017 0.206516409
C   3.539714603 -0.9513492883 -0.0423743251
C   -1.2892244623 -0.3201350659 0.178268639
C   0.1626547981 1.601637467 -0.1432067191
C   -1.094376738 1.080552585 -0.0035420782
C   2.6285222929 1.2789324974 -0.2538351213
C   2.2779855606 -1.4775418628 0.0976633787
C   1.3148682553 0.7685076619 -0.112225737
C   1.133255225 -0.6386370002 0.0673025448
C   -2.6255804039 -0.8950244064 0.3427409195
C   -4.8613534202 0.4490275384 0.5319987218
C   -3.7707293302 -0.231896156 0.3133457752
H   4.7182309799 0.8424189608 -0.3292011187
H   -0.3127829333 -2.2171552134 0.3406848292
H   4.4058317397 -1.603049824 -0.0175392785
H   0.2957855625 2.6695796129 -0.2824282136
H   -1.9615121089 1.7300243229 -0.0326005969
H   2.7629443913 2.3469994616 -0.3902593249
H   2.140791899 -2.5453262961 0.2333449753
H   -2.6757052484 -1.9771450066 0.4486507682
H   -5.5489430404 0.7185291699 -0.2615885092
H   -5.11455657 0.7655256172 1.5412174422
H   -4.0835297514 -0.6113502345 -1.7575938286
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  500.7306
WellDepth[kcal/mol]  58.13
WellDepth[kcal/mol]  3.37
End
Frequencies[1/cm]  65
47.6557          85.2762
110.5325         137.5091          183.2667
254.4873         284.0922          373.2322
383.3305         404.4625          413.4310
427.1121         483.5446          503.6452
525.5981         599.3716          609.1604
644.5790         685.7759          761.2275
767.5694         782.0567          784.0150
835.9268         871.8041          888.9631
891.7821         895.8046          919.4966
964.8807         966.7452          985.1021
996.7166         1009.3820         1042.6344
1094.6169        1150.5578          1174.4815
1179.9030        1197.2920          1241.5470
1281.7074        1289.4384          1327.8247
1393.1864        1398.3897          1413.5533
1458.3294        1481.7288          1503.4538

```

```

1543.4078          1607.9909          1641.1639
1664.3641          1982.7975          3110.0526
3123.2332          3156.1935          3158.5898
3161.0835          3164.1597          3175.6998
3185.1014          3188.4279          3192.0679
ZeroEnergy[kcal/mol] -3.87
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts14-p5-----
Barrier      ts14-p5  i14  p5
RRHO
Geometry[angstrom] 24
C   -3.7006996718 0.459886483 0.0768176268
C    0.2225030897 -1.121154173 -0.068785298
C   -3.5068556878 -0.939719976 0.0256416308
C    1.3187265175 -0.283849154 -0.0648231172
C   -0.1534246469 1.6437441538 0.0305525446
C    1.111888968 1.1224979334 -0.0162025219
C   -2.6195967402 1.3090930962 0.0792347463
C   -2.2374050245 -1.463651412 -0.0218478524
C   -1.2974988004 0.8008471187 0.0310678402
C   -1.1002134688 -0.614362694 -0.0202641297
C    2.6818347582 -0.861209845 -0.1087571485
C    4.9143658784 0.4717882255 0.2385615272
C    3.8002221262 -0.1876530465 0.133598917
H   -4.7074667793 0.860399578 0.1138955162
H    0.3655001602 -2.1965403764 -0.1140279636
H   -4.3671409224 -1.5996052412 0.0236682876
H   -0.2972818636 2.7186957887 0.0674532692
H    1.9731792802 1.7805748493 -0.0160351039
H   -2.765748666 2.3836386144 0.117907282
H   -2.0883700685 -2.5377086581 -0.0619484471
H    2.740514863 -1.9469482194 -0.0824859129
H    2.8253553792 -1.0988441689 -2.0142144548
H    5.454303015 0.80883063 -0.645162875
H    5.3541113045 0.7105224936 1.203796637
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 717.5388
WellDepth[kcal/mol] 34.68
WellDepth[kcal/mol] 5.39
End
Frequencies[1/cm] 65
42.7687          100.0024
116.5452          182.0797          222.2443
251.0710          268.1260          369.5522
383.0397          407.9560          410.2979
464.0060          485.2776          507.5019
526.1080          586.5718          608.2310
644.3548          678.5813          761.0165

```

765.4852	782.4542	784.4510
835.2266	873.7566	883.8304
886.9472	907.2581	955.2278
964.8236	967.1568	982.8166
995.6373	996.4339	1042.3969
1086.0679	1150.4375	1173.8510
1180.7377	1192.5428	1238.9812
1278.6955	1288.9328	1320.3166
1393.2198	1397.1820	1410.4812
1452.3378	1479.5000	1504.2094
1545.2929	1610.7479	1643.6301
1668.5182	1979.6187	3087.7720
3127.5976	3155.8410	3157.8430
3158.1680	3160.7331	3163.7437
3175.3896	3183.6475	3188.1502

ZeroEnergy[kcal/mol] -1.85

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts14-p6-----

Barrier ts14-p6 i14 p6

RRHO

Geometry[angstrom] 24

C	-3.665301	0.426868	0.288838
C	0.245669	-1.108675	-0.239035
C	-3.450897	-0.970833	0.292792
C	1.311310	-0.258726	-0.414552
C	-0.173803	1.652802	-0.245336
C	1.087790	1.143283	-0.414048
C	-2.609477	1.288831	0.114358
C	-2.185887	-1.479576	0.122096
C	-1.291623	0.795913	-0.064367
C	-1.074540	-0.616801	-0.060727
C	2.715577	-0.803206	-0.634902
C	4.561672	0.147183	1.036704
C	3.699283	-0.314026	0.326861
H	-4.668321	0.815341	0.424559
H	0.402674	-2.183234	-0.233529
H	-4.291779	-1.641024	0.431569
H	-0.332500	2.726229	-0.247084
H	1.931839	1.812489	-0.540645
H	-2.771190	2.361802	0.111328
H	-2.021051	-2.552120	0.125470
H	2.693149	-1.896820	-0.602991
H	3.059086	-0.533390	-1.643168
H	5.221754	0.454269	1.811200
H	5.757696	1.218238	-0.288805

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 450.6795

WellDepth[kcal/mol] 37.63

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WellDepth[kcal/mol]  3.35
End
Frequencies[1/cm]   65
23.0358              43.3061
77.1121              143.5213              180.8725
215.6388             250.6938              290.0201
366.9439             402.0135              407.3253
411.0428             485.9321              503.9890
526.6255             577.6872              635.5863
658.3751             667.8629              737.4287
752.2448             765.0766              781.3207
786.5692             832.8690              868.9186
878.5749             903.0521              941.7408
958.8030             966.0046              980.7192
985.1612             997.3401             1042.6079
1148.1454            1172.7595             1179.1794
1188.7823            1213.4614             1238.5026
1277.1847            1289.1681             1322.2129
1392.5186            1397.1355             1408.2386
1461.3924            1474.6256             1503.1973
1546.1495            1613.0883             1646.3885
1674.1010            2170.9902             2997.7885
3055.9136            3153.9269             3158.0270
3160.4406            3163.5144             3175.5814
3179.6240            3188.3237             3463.2031
ZeroEnergy[kcal/mol]  1.1
ElectronicLevels[1/cm] 1
0  2
End
!-----
!-----bar_ts2-p4-----
Barrier      ts2-p4  i2  p4
RRHO
Geometry[angstrom]  24
C   -3.9020997809  0.2518136142 -0.0488626414
C    0.1947809317 -0.7950470074  0.0744444134
C   -3.5232082297 -1.1075865264  0.0453710048
C    1.1731976037  0.1803459961  0.0238456178
C   -0.5453529917  1.8972738776 -0.1117533893
C    0.7781465902  1.5505298235 -0.0711355949
C   -2.9447922606  1.2367210887 -0.1006697586
C   -2.1951889477 -1.4561389203  0.085965346
C   -1.5658762768  0.9107770484 -0.0607558918
C   -1.181086136  -0.4633006839  0.0344739606
C    2.5770100181 -0.1178816178  0.0672593491
C    3.7894124901 -0.0124709791  0.1046758511
C    5.2385880491 -0.1021591758  0.1486882169
H   -4.9537245897  0.5136497042 -0.0801175676
H    0.4874348821 -1.8362983541  0.145223437
H   -4.2879648048 -1.8749937328  0.0853931494
H   -0.8298544407  2.9418534365 -0.1842607142
H    1.5484002863  2.3109411586 -0.1105104358
H   -3.2341859092  2.2800262842 -0.1730215343
H   -1.9023487045 -2.4982522787  0.1580729554

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H    2.6136624354 -2.1234064065 0.0321745949
H    5.6404529314 0.3788701268 1.0455004212
H    5.6939306305 0.3762658804 -0.7235357686
H    5.5531362236 -1.1516853564 0.159890979
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 558.1328
WellDepth[kcal/mol] 35.51
WellDepth[kcal/mol] 5.08
End
Frequencies[1/cm] 65
19.9912          68.5063
93.1169          97.0580          170.4822
182.4707        266.4483          284.8931
337.4801        395.9449          397.9627
444.5423        484.9825          518.7388
525.6564        554.8158          581.7702
617.0338        660.2545          668.3550
761.0202        780.3007          781.6594
832.6040        855.5958          876.7714
921.7636        953.3995          966.0228
979.4538        997.9412        1017.4385
1041.9349       1043.1509        1052.1448
1152.2320       1173.3088        1179.0925
1209.1156       1243.5111        1282.7710
1291.4211       1374.4422        1394.5864
1406.2107       1412.8189        1464.0474
1470.6395       1476.0896        1501.0236
1535.3366       1604.8772        1641.7016
1667.2802       2248.1687        3013.6115
3069.5251       3077.6418        3157.8036
3162.4745       3164.2868        3173.7743
3176.1097       3188.3850        3192.9934
ZeroEnergy[kcal/mol] -4.54
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts2-p5-----
Barrier      ts2-p5  i2  p5
RRHO
Geometry[angstrom] 24
C            -3.758652      0.450192      0.000004
C             0.165116     -1.136492     -0.000003
C            -3.565308     -0.950229      0.000004
C             1.264976     -0.300905     -0.000004
C            -0.209363      1.630692     -0.000003
C             1.055457      1.108402     -0.000004
C            -2.676547      1.298557      0.000001
C            -2.295604     -1.476035      0.000001
C            -1.354738      0.788413     -0.000001
C            -1.157696     -0.627760     -0.000001

```

C	2.618742	-0.877437	-0.000004
C	3.748950	-0.216297	0.000001
C	4.913022	0.385477	0.000008
H	-4.765473	0.852246	0.000005
H	0.307448	-2.212952	-0.000003
H	-4.426056	-1.609520	0.000005
H	-0.353262	2.706317	-0.000003
H	1.917258	1.766154	-0.000006
H	-2.822195	2.373871	0.000001
H	-2.147055	-2.550920	0.000001
H	2.676951	-1.965726	-0.000008
H	5.385854	0.700969	0.925771
H	5.385861	0.700978	-0.925750
H	6.350538	-1.220885	0.000006

Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 364.4727
 WellDepth[kcal/mol] 35.69
 WellDepth[kcal/mol] 2.88
 End
 Frequencies[1/cm] 65

45.8409	93.7806	
118.9777	168.8815	183.6629
218.6258	266.4369	289.1780
360.9017	387.4330	402.5178
421.3181	484.0472	509.5588
526.0192	605.1940	612.8658
644.4237	694.4512	762.6646
763.7477	782.1298	784.1393
835.4413	873.3269	887.3219
896.5254	897.0431	921.9579
964.3822	966.7676	982.5125
996.4094	1017.2344	1042.6303
1091.0918	1150.7966	1174.1896
1180.0138	1196.0201	1240.3339
1279.8506	1289.0112	1323.7799
1393.0392	1397.3946	1412.7416
1460.2518	1481.2507	1505.3257
1543.8836	1609.8265	1643.4395
1667.6830	2000.1882	3105.2836
3109.1033	3155.8287	3158.2324
3160.1051	3163.5986	3175.4678
3180.3865	3181.3439	3188.2396

ZeroEnergy[kcal/mol] -4.36
 ElectronicLevels[1/cm] 1
 0 2
 End
 !-----
 !-----bar_tsa-7-----
 Barrier tsa-7 i7 p0a
 RRHO
 Geometry[angstrom] 24

```

C   -4.0000109749  0.4033492002 -0.4659012376
C   -0.0367350294 -0.9925940733  0.1238179299
C   -3.6903460802 -0.9571717598 -0.6964008755
C   0.8911719755 -0.0883163644  0.5317801026
C   -0.6612899427  1.7137689997  0.5862191771
C   0.6257167597  1.261695255  0.7844921381
C   -3.0223550294  1.2747416149 -0.0514365825
C   -2.4102269012 -1.419602457 -0.508506621
C   -1.6888891965  0.8328453842  0.1533865017
C   -1.3772557879 -0.5457537556 -0.0812950446
H   -5.0140129902  0.7555027833 -0.6182281862
H   0.2115953324 -2.0350302603 -0.0511365777
H   -4.4702205032 -1.6359856912 -1.0233140694
H   -0.9066725754  2.7568413428  0.762753119
H   1.4073192655  1.9320798944  1.1241670705
H   -3.258589672  2.3189395608  0.1258756438
H   -2.171836953 -2.4633413023 -0.6849040882
C   3.3185568028 -0.3849476197  2.1125522344
C   3.3065430915 -1.5202479849 -0.2243054859
C   3.1016973696 -0.8782222627  0.9009846148
H   4.0387601981  0.4132090402  2.264454946
H   2.7151229539 -0.6825948091  2.9630029756
H   2.7153919709 -1.3514933305 -1.1143074048
H   4.093290916 -2.2681324047 -0.27542328
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  370.7338
WellDepth[kcal/mol]  64.34
WellDepth[kcal/mol]  2.61
End
      Rotor      Hindered      ! 25 cm^-1
      Group                      18 19 21 22 23 24
      Axis                      4 20
      Symmetry      2
      Potential[kcal/mol]      4
0      0.082433425 0.062369433 0.880468746
      End
Frequencies[1/cm]  64
                  43.2367
75.5997              94.8366              165.6363
181.3044             230.5669              242.4409
372.3333             389.3906              393.6208
477.5358             490.1562              514.3201
515.5837             619.8558              629.9287
746.8745             763.7663              765.9630
775.6131             807.8901              813.1685
827.6224             853.3466              884.7754
891.9249             930.4192              957.8761
969.6901             994.7007             1006.6454
1020.7432            1038.0773             1045.6731
1072.4831            1144.0000             1161.2406
1172.4382            1210.3374             1252.0985

```

1277.2443	1343.8608	1385.6497
1393.7395	1427.1614	1459.1857
1464.5729	1475.4377	1531.6100
1595.7472	1614.8263	1656.9876
1927.9493	3119.6821	3123.7609
3151.0548	3153.4389	3156.9892
3162.4044	3174.2672	3174.7098
3186.7835	3201.1444	3218.0625

ZeroEnergy[kcal/mol] 3.74

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_tsa-14-----

Barrier tsa-14 i14 p0a

RRHO

Geometry[angstrom] 24

C	-1.9710088797	-0.9466165477	0.4306779248
C	1.1959351256	1.7891338222	-0.2715424956
C	-2.2356031472	0.4420268274	0.3890991995
C	2.4410617339	1.2765203027	-0.4517012704
C	1.7154587641	-0.9759124684	-0.1856843299
C	2.745620596	-0.0886533986	-0.4127137875
C	-0.6923308972	-1.4126912569	0.2446953618
C	-1.2177673516	1.3366883096	0.1623214106
C	0.3842337481	-0.5180749075	0.0080776596
C	0.1139396663	0.8883010499	-0.0339010793
H	-2.7831645927	-1.6419879703	0.610260077
H	0.9958493558	2.8566314802	-0.3038299099
H	-3.2488627225	0.7986900812	0.5373145868
H	1.9112644605	-2.0435985584	-0.1512697909
H	3.7616263477	-0.4404131491	-0.5571939067
H	-0.4872408557	-2.4778484983	0.2763707923
H	-1.4204890636	2.4022353139	0.1302347381
C	4.2429634293	2.7581772852	-0.8840468176
C	6.2022085117	2.0387064747	0.7004465884
C	5.2650428174	2.4366880665	-0.1086874157
H	4.2109021539	2.4288297687	-1.9168011999
H	3.5927066754	3.5834087266	-0.6143456439
H	6.0461667943	1.203596124	1.3802700633
H	7.1737653302	2.5248161223	0.7350642451

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 239.2847

WellDepth[kcal/mol] 39.53

WellDepth[kcal/mol] 1.87

End

Rotor	Hindered	! 12 cm ⁻¹
Group		19 20 21 22 23 24
Axis		4 18
Symmetry	1	
Potential[kcal/mol]		8

```

0      0.130493757 0.291590529 0.001067394 0.031020309 0.031012151 0.0346812
0.046290127
End
Frequencies[1/cm]  64
                 33.8973
67.1787          113.9326          177.2693
200.3338          321.2507          343.7576
367.5468          378.6628          388.6248
476.7878          487.5111          496.7706
515.4107          620.1171          628.9492
745.7566          751.1684          766.8062
771.3702          814.1119          847.2915
859.3780          870.2684          872.8879
889.8419          936.8604          957.9717
969.7716          994.6538          999.1959
1031.9700         1038.6551         1047.2935
1069.9930         1145.3106         1161.8744
1173.1998         1211.6244         1254.0434
1277.5746         1345.8875         1386.1275
1393.5996         1420.4004         1460.4570
1465.8396         1469.4568         1531.7856
1596.0864         1615.2271         1657.2332
1974.8042         3094.2402         3124.3435
3141.2065         3149.9294         3156.6926
3161.7556         3162.5280         3169.8006
3174.3456         3187.1507         3200.9196
ZeroEnergy[kcal/mol]  3.0
ElectronicLevels[1/cm] 1
0  2
End
!-----
!-----bar_ts10-19-----
Barrier      ts10-19  i10  i19
RRHO
Geometry[angstrom]  24
C   3.5415655422 0.5283386696 0.2733729652
C  -0.2259627703 -1.3430225814 -0.2112450856
C   3.4561468646 -0.8829936358 0.2219898673
C  -1.3781369885 -0.5919289578 -0.3187504277
C  -0.0620915103 1.4451886333 -0.1081694856
C  -1.2775810347 0.8270625198 -0.2635909044
C   2.4067809566 1.2949609284 0.1664333304
C   2.2386563227 -1.4990984632 0.0643704881
C   1.1336080441 0.6898524102 0.0033112709
C   1.0464922809 -0.7364524395 -0.0492698765
H   4.5087560592 1.0022063251 0.3979478556
H  -0.2856665859 -2.4259598523 -0.2493873093
H   4.3589768496 -1.477233825 0.307848525
H  -0.0032375459 2.5280922446 -0.0669001322
H  -2.1828332748 1.4181952395 -0.3448480862
H   2.4695952522 2.3775908133 0.2058998034
H   2.1721212128 -2.5814538623 0.0249340176
C  -2.7023644831 -1.2365984092 -0.5102657461
C  -3.312386698 -1.4278392428 1.8749855409

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C   -3.5570950851 -1.5960873129 0.5257641781
H   -3.0199044303 -1.4243458817 -1.5324897277
H   -4.0387751364 -1.7370653649 2.6155820568
H   -2.3901904109 -0.9843338105 2.230277194
H   -4.5026204307 -2.0513101447 0.2391216883
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 69.8626
WellDepth[kcal/mol] 2.9
WellDepth[kcal/mol] 3.1
End
Frequencies[1/cm] 65
67.8243          157.5799
173.8269          175.4641          298.4633
326.1858          398.5906          403.4319
444.2652          485.4007          505.6832
521.8203          525.4738          598.6160
634.6266          667.9718          697.4769
738.1726          769.5193          780.6064
789.7737          809.6093          835.5701
872.8868          900.1543          919.7046
963.4460          970.8201          977.8654
994.6662          995.5600         1027.9459
1041.3933         1112.2176         1153.1265
1170.4738         1177.8639         1194.9317
1221.7119         1243.1394         1275.9898
1288.7286         1364.4843         1390.7664
1398.2672         1425.2334         1447.9288
1461.6116         1501.8120         1520.7968
1536.8603         1603.8413         1640.6813
1668.9666         3126.5557         3143.3211
3150.0833         3156.5052         3158.7634
3161.5035         3164.5559         3174.6728
3180.8674         3187.2827         3240.7940
ZeroEnergy[kcal/mol] -59.1
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts19-20-----
Barrier      ts19-20  i19  i20
RRHO
Geometry[angstrom] 24
C   3.647561846 0.4742217112 -0.0683128381
C   -0.1900111136 -1.2428831077 0.5713021381
C   3.5402275859 -0.8338738872 0.4468775145
C   -1.3460372568 -0.4600387513 0.2832909219
C   0.0388804033 1.416453359 -0.3736958093
C   -1.2111349783 0.8585592113 -0.1719907623
C   2.5151136907 1.2052175852 -0.3500542077
C   2.2961116209 -1.3897685978 0.6600836017
C   1.2230286832 0.6614184698 -0.1410424807

```

```

C   1.1175237974 -0.6739143666 0.3601843735
C   -2.5724928599 -1.2530473695 0.2090619345
C   -1.0021588934 -2.8679854125 -0.6539121014
C   -2.3731052131 -2.5050053367 -0.2473524862
H   4.6276836859 0.9066101794 -0.2365727672
H   -0.2701715624 -2.0070908108 1.3365869438
H   4.4364440226 -1.3991801317 0.6756597957
H   0.1309331789 2.4361770607 -0.7308996052
H   -2.1027800908 1.4297632635 -0.4093134374
H   2.59921526 2.2159468708 -0.7359448562
H   2.2097756921 -2.3980617937 1.0524741486
H   -3.5514684428 -0.8453521087 0.4357719172
H   -0.6090836016 -3.8421234182 -0.3743216485
H   -0.656995998 -2.5091501384 -1.6205425886
H   -3.1876304563 -3.2219034798 -0.3258647006
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 638.8802
WellDepth[kcal/mol] 29.22
WellDepth[kcal/mol] 31.74
End
Frequencies[1/cm] 65
99.4242          107.1809
167.1875          221.8877          266.6939
356.0410          410.7650          429.5283
455.5837          487.7448          518.9563
541.0534          556.3296          613.4703
653.6072          674.5092          711.8163
731.6470          750.3336          774.4498
786.7626          802.8058          828.5291
877.8900          889.1340          942.1589
955.2309          956.4267          962.3481
975.4885          989.7994         1009.0763
1046.2136         1061.0969         1132.1317
1154.9764         1158.3829         1175.3983
1196.1748         1227.4254         1261.9997
1283.5966         1334.7080         1365.5998
1373.5134         1390.1160         1450.4765
1453.0605         1487.8586         1534.7365
1561.4917         1589.8197         1610.4898
1645.8394         3095.9836         3126.8734
3145.0017         3155.8541         3158.1965
3160.7622         3173.8081         3177.1672
3177.8425         3179.3364         3187.4929
ZeroEnergy[kcal/mol] -32.98
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts20-p3-----
Barrier      ts20-p3  i20  p3
RRHO

```

```

Geometry[angstrom]    24
C    3.6199469131 0.4847184479 0.0398827217
C   -0.2668666042 -1.2105180837 0.0730829471
C    3.4727822653 -0.9169862608 0.1301720974
C   -1.3752133056 -0.3744111308 -0.1384633342
C    0.0458975145 1.5594576995 -0.1726072525
C   -1.2189194353 1.0236567708 -0.2306178432
C    2.5091003313 1.2903794219 -0.0478438886
C    2.2203001493 -1.4868341109 0.1373585158
C    1.2034872791 0.7377878694 -0.0523311489
C    1.0580473972 -0.6840765418 0.0474282532
C   -2.5705671344 -1.2053947201 -0.2458517453
C   -0.7319891516 -2.6494565398 -0.0260095753
C   -2.226414709 -2.5042539886 -0.1737677195
H    4.6117977494 0.9222579997 0.0396901635
H   -0.4449688671 -1.140227121 2.0482195302
H    4.353994101 -1.545183066 0.197556559
H    0.1843971033 2.6332552076 -0.2438399718
H   -2.0839624148 1.6650645803 -0.3586987705
H    2.6189805435 2.3676102889 -0.1193916885
H    2.1149463933 -2.5629224648 0.2179732322
H   -3.5739525608 -0.8175536304 -0.3678706685
H   -0.4531628582 -3.2639330328 0.8353147178
H   -0.2994482909 -3.133923589 -0.91213115
H   -2.9022024086 -3.3477480054 -0.2201399811
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 629.0042
WellDepth[kcal/mol] 32.58
WellDepth[kcal/mol] 4.19
End
Frequencies[1/cm] 65
114.2836      133.5814
233.9749      238.8545      255.4998
376.7410      399.8687      425.0452
432.8509      444.1231      480.3414
521.0521      529.5830      553.3525
618.1347      673.7523      684.4805
720.3311      751.2028      761.9177
792.1620      830.7460      839.3761
868.7640      876.4799      933.3138
955.7548      958.0825      960.3169
971.3406      984.5602      992.7733
1046.1015     1059.9232      1118.6689
1149.6490     1165.8012      1178.8203
1183.7411     1233.7718      1246.1699
1267.3775     1289.7339      1357.1926
1372.8745     1394.7314      1407.6994
1436.2232     1464.2200      1481.3264
1551.6801     1575.3398      1609.3041
1627.9994     1657.6823      3011.3370
3062.2763     3157.7390      3160.7227

```

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3165.7743          3177.8975          3178.8533
3188.7192          3193.0592          3216.6704
ZeroEnergy[kcal/mol] -32.14
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----bar_ts9-p5-----
Barrier      ts9-p5  i9  p5
RRHO
Geometry[angstrom] 24
C 3.7230963898 0.3981884795 0.1045934107
C -0.216180129 -1.1175823297 -0.1884371107
C 3.5151860596 -0.9733334296 -0.1676603909
C -1.3088632159 -0.2865729714 -0.0170807913
C 0.18677235 1.5929910821 0.3501019211
C -1.083631181 1.0948264111 0.2548604106
C 2.6500150916 1.2413097881 0.2750336787
C 2.2399992557 -1.4763172288 -0.2643822681
C 1.3231311327 0.7544945998 0.181955641
C 1.1111540402 -0.6327620513 -0.0934616396
C -2.6606909348 -0.8410031893 -0.109626281
C -4.8845183661 0.4499800769 0.3688468306
C -3.7925025814 -0.1648290416 0.0076824997
H 4.7340862502 0.7826144415 0.1783233404
H -0.3709009592 -2.171364307 -0.399563067
H 4.3689319656 -1.6282897929 -0.3004737177
H 0.343134266 2.6469077092 0.5560571035
H -1.9381712902 1.7489997033 0.3829223818
H 2.8074994988 2.2944400198 0.4837518173
H 2.0797967047 -2.5288606624 -0.4738640978
H -2.7324035411 -1.9007820247 -0.3471977539
H -5.5193148677 0.9731901762 -0.3371813665
H -5.1933610988 0.4474609274 1.4116388906
H -3.9857548395 0.1236356139 -2.0923104416
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 500.7546
WellDepth[kcal/mol] 61.82
WellDepth[kcal/mol] 3.37
End
Frequencies[1/cm] 65
47.6575          85.2753
110.5319         137.5114         183.2656
254.4871         284.0916         373.2378
383.3285         404.4638         413.4317
427.1200         483.5448         503.6453
525.5979         599.3704         609.1608
644.5793         685.7748         761.2283
767.5703         782.0584         784.0121
835.9263         871.8056         888.9636
891.7817         895.8024         919.4968

```

964.8809	966.7458	985.1017
996.7165	1009.3821	1042.6348
1094.6155	1150.5576	1174.4822
1179.9034	1197.2921	1241.5485
1281.7073	1289.4390	1327.8259
1393.1880	1398.3901	1413.5540
1458.3241	1481.7277	1503.4535
1543.4082	1607.9912	1641.1641
1664.3633	1982.7973	3110.0547
3123.2356	3156.1934	3158.5940
3161.0843	3164.1602	3175.6998
3185.1052	3188.4277	3192.0692

ZeroEnergy[kcal/mol] -3.87

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----bar_ts0-8-----

Barrier ts0-8 i8 p0p

RRHO

Geometry[angstrom] 24

```

C 3.8633115301 -0.0440794168 0.4589066793
C -0.1956131419 -0.7757107773 -0.5388711269
C 3.4331506641 -1.3620297341 0.1795217729
C -1.0414716307 0.2880749698 -0.5628159708
C 0.668462941 1.8448319925 0.0146385202
C -0.6504672173 1.6087075605 -0.3092268926
C 2.9716528658 0.9996604004 0.408381422
C 2.1210308113 -1.6102190511 -0.1440281117
C 1.608394198 0.7810114319 0.0780979564
C 1.1742369898 -0.5549596173 -0.2040016007
H 4.9013193597 0.1385398753 0.7131708494
H -0.5321951423 -1.7831201044 -0.7661123371
H 4.1457055042 -2.1783558897 0.2218830273
H 1.007673679 2.8552741353 0.223363542
H -1.3620721668 2.4258458162 -0.365116992
H 3.3006028557 2.0116177142 0.6217135451
H 1.7903092524 -2.6211873369 -0.358771022
C -3.2751057825 -0.066080178 -2.3254303348
C -3.785972882 -0.1910688378 0.2627838996
C -3.2600711642 -0.0820984077 -1.1056494094
H -3.0630822686 -0.0142089083 -3.3662440418
H -4.8656251739 -0.3611160585 0.2330390177
H -3.5921150827 0.7205690926 0.8324180175
H -3.3154969982 -1.0178686707 0.7991515905

```

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 364.7857

WellDepth[kcal/mol] 41.71

WellDepth[kcal/mol] 3.46

End

Rotor Hindered ! 158 cm⁻¹ CH3

```

      Group                22 23 24
      Axis                19 20
      Symmetry            3
      Potential[kcal/mol] 4
0    0.67872755 1.281321244 0.644327475
      End
      Rotor      Hindered      ! 22 cm^-1
      Group                18 19 21 22 23 24
      Axis                4 20
      Symmetry            1
      Potential[kcal/mol] 8
0    0.004344876 1.044571916 0.368266553 0.041007124 0.520076811 0.745740554
      0.385257003
      End
Frequencies[1/cm] 63
                  44.1099
66.9173          152.6870
179.4465          224.6088          245.0673
360.6165          382.9342          390.1903
478.8857          491.0492          509.9220
515.8088          571.6787          623.9236
631.3283          679.4860          747.2507
766.8444          768.2011          781.7072
812.9915          854.3476          892.4799
917.9061          935.0115          957.4057
969.2578          994.7451        1029.4248
1041.5414         1053.8436        1065.4472
1144.9833         1162.1065        1172.9189
1210.9202         1253.9223        1277.7853
1346.1862         1385.5650        1393.6082
1414.4197         1459.3954        1467.7252
1477.0597         1481.2383        1531.2536
1596.1948         1614.1237        1657.1665
2070.3004         3033.7439        3097.6832
3100.8197         3146.7032        3147.9644
3155.6171         3160.5144        3167.2053
3173.3798         3186.3646        3454.9822
ZeroEnergy[kcal/mol] 3.46
ElectronicLevels[1/cm] 1
0 2
End
!-----

!-----bar_ts8-p7-----
Barrier      ts8-p7  i8  p7
RRHO
Geometry[angstrom] 24
C          -3.607398      0.177020      0.152335
C           0.460048     -0.951104     -0.151188
C          -3.247648     -1.189527      0.213804
C           1.441269      0.007563     -0.310815
C          -0.244628      1.753846     -0.273876
C           1.070530      1.381312     -0.366920
C          -2.641319      1.141496     -0.005446

```

C	-1.929975	-1.565153	0.116598
C	-1.272109	0.787733	-0.108779
C	-0.907222	-0.593792	-0.046290
C	3.778198	-0.850127	-1.064184
C	2.833363	-0.377225	-0.435119
C	3.540936	0.188144	1.635808
H	-4.651026	0.460175	0.230020
H	0.737239	-1.998382	-0.109269
H	-4.019142	-1.941098	0.337834
H	-0.516729	2.802833	-0.327641
H	1.845292	2.127387	-0.496294
H	-2.915632	2.190252	-0.053746
H	-1.652781	-2.613097	0.162854
H	4.746340	-1.198606	-1.337691
H	2.885754	-0.458225	2.206385
H	3.306610	1.245493	1.639920
H	4.589797	-0.077848	1.612070

Core RigidRotor
 SymmetryFactor 0.5
 End
 Tunneling Eckart
 ImaginaryFrequency[1/cm] 532.2373
 WellDepth[kcal/mol] 34.3
 WellDepth[kcal/mol] 11.3
 End
 Frequencies[1/cm] 65

	27.7948	70.6610
77.6506	136.2543	154.8382
182.8958	239.8253	340.6894
356.8632	409.6971	409.9841
477.4442	485.2458	512.6473
521.5793	535.5788	559.8827
580.7187	633.6376	659.6130
688.4179	696.3183	759.1767
780.2217	782.3936	832.5819
873.5417	878.7338	902.0204
916.0132	964.9340	970.4237
980.3804	996.9217	1042.1040
1141.4150	1171.4461	1174.5510
1179.7892	1229.6648	1273.2195
1288.7322	1369.7715	1393.8886
1401.8953	1416.5141	1421.1694
1465.1758	1497.2007	1538.4098
1604.4867	1639.6767	1666.9434
1997.4584	3087.3002	3157.8222
3162.1219	3164.2455	3175.2643
3177.4559	3188.0410	3189.1667
3246.8920	3249.0233	3436.0875

ZeroEnergy[kcal/mol] -4.
 ElectronicLevels[1/cm] 1
 0 2
 End
 !-----
 End

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