

Hydrogenation of phenyl substituted C≡N, C=N, C≡C, C=C and C=O functional groups by Chromium, Molybdenum and Tungsten
PNP pincer complexes – A DFT Study

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Table S1. Gibbs free energy barriers and reaction free energy (in parenthesis) for catalyst interconversion as well as benzonitrile hydrogenation (kJ/mol) in gas phase and THF solution

	H ₂ addition (1M + H ₂ = 2M)		Ph-CN hydrogenation	
	Gas	THF	Gas	THF
2Cr-cis	98.1 (20.6)	91.9 (-5.8)	82.6 (-37.4)	123.8 (-13.0)
2Cr-trans	106.2 (10.7)	100.2 (-15.2)	90.4 (-27.4)	109.4 (-10.2)
2Mo-cis	95.4 (14.8)	94.9 (-10.7)	74.3 (-31.6)	96.5 (-14.7)
2Mo-trans	104.9 (16.8)	105.9 (-7.4)	79.2 (-33.5)	100.7 (-18.1)
2W-cis	100.9 (13.8)	102.7 (-10.1)	78.6 (-30.6)	101.2 (-15.3)
2W-trans	111.9 (16.5)	115.8 (-5.6)	85.1 (-33.3)	105.4 (-19.8)

Table S2. Relative energies (kJ/mol) of M-PNP (**1**) and H-M-PN^HP (**2M**) isomers in C_s and C₁ symmetrical geometries

M-PNP (1M)			
Symmetry	Cr	Mo	W
<i>cis</i> -C _s	6.5	9.4	10.2
<i>trans</i> -C _s	1.5	4.1	4.8
<i>syn</i> -C ₁	0.0	0.0	0.0
<i>anti</i> -C ₁	1.6	2.2	1.5
H-M-PN ^H P (2M)			
	Cr	Mo	W
<i>cis</i> -C _s	10.0	0.0	0.0
<i>trans</i> -C _s	0.0	2.0	2.7
<i>syn</i> -C ₁	21.3	13.0	13.0
<i>anti</i> -C ₁	3.8	8.1	9.8

Table S3. Computed bond lengths (Å) of M-PNP (**1M**) and H-M-PN^HP (**2**)

	1Cr-cis	1Mo-cis	1W-cis
M-N	1.935	2.083 [2.055 ^a]	2.063 [2.061 ^a]
M-P	2.343	2.486	2.472
M-L ₁	1.657	1.812 [1.856 ^a]	1.813 [1.882 ^a]
M-L ₂	1.842	1.968 [1.896 ^a]	1.963 [1.869 ^a]
	1Cr-trans	1Mo-trans	1W-trans
M-N	1.943	2.086 [2.055 ^a]	2.065 [2.061 ^a]
M-P	2.338	2.478	2.467
M-L ₁	1.812	1.952 [1.896 ^a]	1.951 [1.869 ^a]
M-L ₂	1.672	1.822 [1.856 ^a]	1.820 [1.882 ^a]
	2Cr-cis	2Mo-cis	2W-cis
M-N	2.230	2.343	2.328
M-P	2.320	2.465	2.455
M-L ₁	1.659	1.809	1.810
M-L ₂	1.842	2.008	1.991
M-H	1.661	1.817	1.819
N-H	1.016	1.017	1.018
	2Cr-trans	2Mo-trans	2W-trans
M-N	2.196	2.324	2.310
M-P	2.323	2.463	2.452
M-L ₁	1.822	1.975	1.971
M-L ₂	1.672	1.837	1.831
M-H	1.677	1.836	1.840
N-H	1.017	1.018	1.018

^a Experimental values from *Chem. Asian J.* **2014**, *9*, 328-337.

Table S4. Natural charge (δ/e), natural bond orbitals and atomic hybrid contributions for the σ and π bonds of M-PNP (**1**).

		1Cr-cis	1Mo-cis	1W-cis
δ/e	M	-1.156	-0.784	-0.598
	N	-0.465	-0.540	-0.566
N-M	σ	18.62%; Cr[sp ^{2.2} d ^{2.2}] 81.38%; N[sp ^{1.28}]	17.80%; Mo[sp ^{2.78} d ^{2.73}] 82.20%; N[sp ^{1.24}]	18.21%; W[sp ^{2.91} d ^{2.85}] 81.79%; N[sp ^{1.15}]
	π	15.40%; Cr[pd ^{1.19}] 84.60%; N[p]	13.81%; Mo[p ^{1.05} d] 86.19%; N[p]	13.74%; W[p ^{1.09} d] 86.26%; N[p]
M-NO	σ	25.24%; Cr[sp ^{1.77} d ^{2.13}] 74.76%; N[sp ^{0.57} d ^{0.03}]	22.34%; Mo[sp ^{1.94} d ^{2.13}] 77.66%; N[sp ^{0.53} d ^{0.01}]	22.52%; W[sp ^{1.91} d ^{2.18}] 77.48%; N[sp ^{0.48}]
	π	52.47%; Cr[pd ^{9.4}] 47.53%; N[p]	49.74%; Mo[pd ^{15.28}] 50.26%; N[p]	46.19%; W[pd ^{16.42}] 53.81%; N[p]
	π	64.41%; Cr[pd ^{2.53}] 35.59%; N[sp ^{10.48} d ^{5.17}]	62.87%; Mo[pd ^{3.21}] 37.13%; N[sp ^{16.89} d ^{5.79}]	39.62%; W[pd ^{3.18}] 60.38%; N[p]
		1Cr-trans	1Mo-trans	1W-trans
δ/e	M	-1.182	-0.813	-0.620
	N	-0.466	-0.537	-0.563
N-M	σ	17.92%; Cr[sp ^{2.66} d ^{2.22}] 82.08%; N[sp ^{1.29}]	17.41%; Mo[sp ^{3.20} d ^{2.80}] 82.59%; N[sp ^{1.23}]	17.82%; W[sp ^{3.24} d ^{2.85}] 82.18%; N[sp ^{1.14}]
	π	15.89%; Cr[sp ^{57.50} d ^{85.16}] 84.11%; N[p]	14.28%; Mo[pd ^{1.06}] 85.72%; N[p]	14.23%; W[pd ^{1.02}] 85.77%; N[p]
M-NO	σ	23.12%; Cr[sp ^{2.39} d ^{1.99}] 76.88%; N[sp ^{0.55}]	21.60%; Mo[sp ^{2.36} d ^{2.25}] 78.40%; N[sp ^{0.48}]	22.00%; W[sp ^{2.27} d ^{2.26}] 78.00%; N[sp ^{0.49}]
	π	54.59%; Cr[pd ^{12.37}] 45.41%; N[p]	50.78%; Mo[pd ^{19.62}] 49.22%; N[p]	46.96%; W[pd ^{21.32}] 53.04%; N[p]
	π	42.59%; Cr[pd ^{2.35}] 57.41%; N[p]	40.68%; Mo[pd ^{2.83}] 59.32%; N[p]	38.91%; W[pd ^{2.91}] 61.09%; N[p]

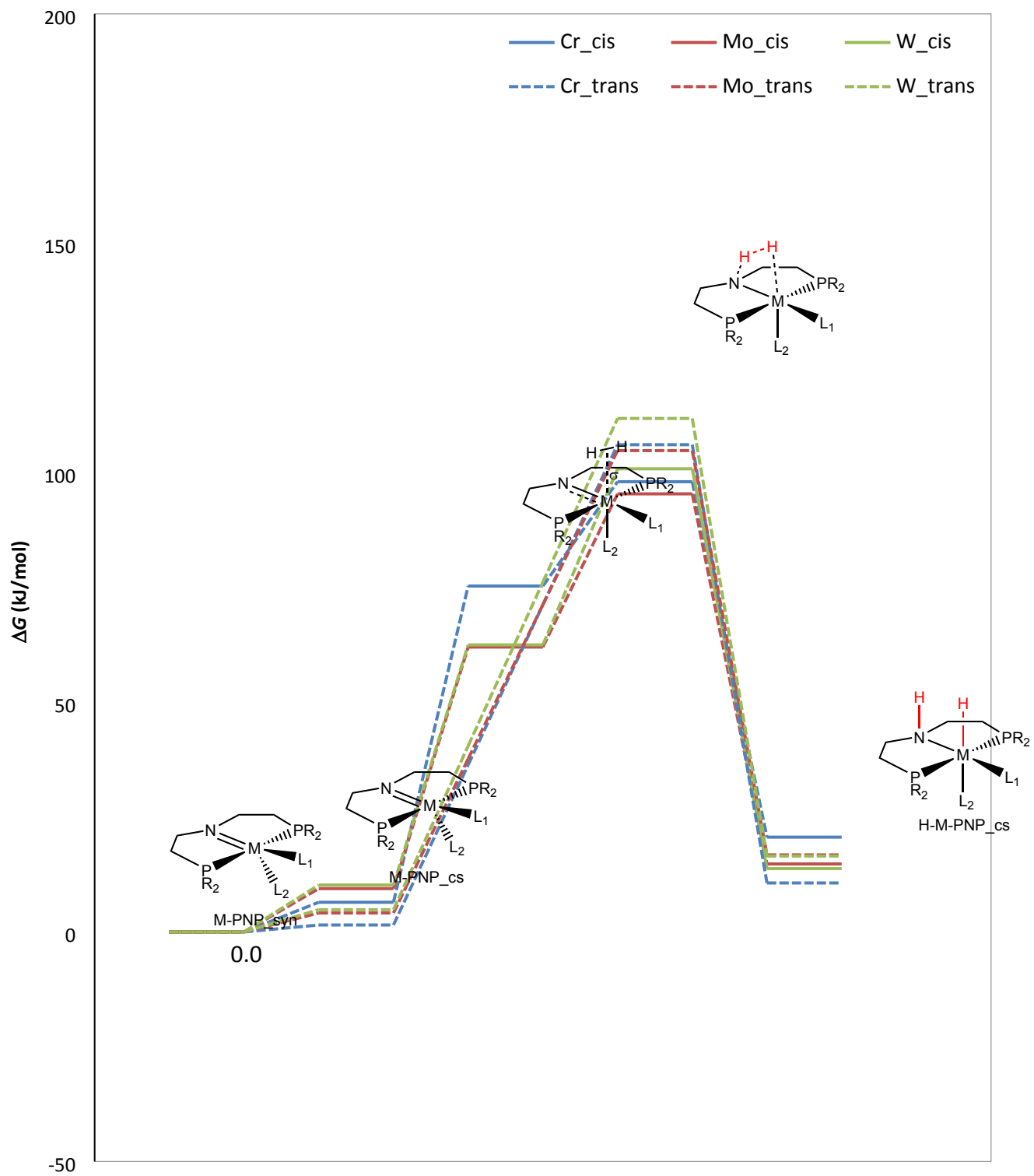
Table S5. Natural charge (δ/e), natural bond orbitals and atomic hybrid contributions for the σ and π bonds of H-M-PN^HP(2M).

		2Cr-cis	2Mo-cis	2W-cis
δ/e	M	-1.713	-1.416	-1.236
	H _M	-0.026	-0.076	-0.088
	N	-0.496	-0.519	-0.524
	H _N	+0.403	+0.406	+0.407
M-H	σ	44.53%; Cr[sp ^{2.86} d ^{2.23}] 55.47%; H[s]	42.74%; Mo[sp ^{3.31} d ^{2.21}] 57.26%; H[s]	42.95%; W[sp ^{3.82} d ^{2.51}] 57.05%; H[s]
M-P	σ	30.45%; Cr[sp ^{2.06} d ^{1.96}] 69.55%; P[sp ^{1.61}]	29.95%; Mo[sp ^{2.14} d ^{1.80}] 70.05%; P[sp ^{1.59}]	31.70%; W[sp ^{2.39} d ^{2.11}] 68.30%; P[sp ^{1.57}]
N-H	σ	70.72%; N[sp ^{4.23}] 29.28%; H[s]	70.96%; N[sp ^{4.50}] 29.04%; H[s]	70.80%; N[sp ^{2.71}] 29.20%; H[s]
N-M	σ	12.69%; Cr[sp ^{7.06} d ^{6.55}] 87.31%; N[sp ^{2.80}]	12.61%; Mo[sp ^{9.65} d ^{7.21}] 87.39%; N[sp ^{2.45}]	LP N
M-NO	σ	24.78%; Cr[sp ^{3.07} d ^{2.55}] 75.22%; N[sp ^{0.58}]	22.79%; Mo[sp ^{2.52} d ^{2.39}] 77.21%; N[sp ^{0.49}]	24.82%; W[sp ^{0.76} d ^{2.50}] 75.18%; N[sp ^{0.49}]
	π	54.06%; Cr[pd ^{12.46}] 45.94%; N[p]	50.20%; Mo[pd ^{14.47}] 49.80%; N[p]	46.78%; W[pd ^{14.56}] 53.22%; N[p]
	π	52.21%; Cr[pd ^{8.14}] 47.79%; N[p]	69.52%; Mo[pd ^{13.61}] 30.48%; N[p ^{3.58} d]	46.19%; W[pd ^{15.60}] 53.81%; N[p]
		2Cr-trans	2Mo-trans	2W-trans
δ/e	M	-1.703	-1.414	-1.226
	H _M	+0.001	-0.075	-0.097
	N	-0.488	-0.509	-0.515
	H _N	+0.395	+0.400	+0.402
M-H	σ	43.79%; Cr[sp ^{4.74} d ^{2.83}] 56.21%; H[s]	41.79%; Mo[sp ^{5.09} d ^{2.66}] 58.21%; H[s]	41.41%; W[sp ^{5.21} d ^{2.56}] 58.59%; H[s]
M-P	σ	29.11%; Cr[sp ^{2.31} d ^{1.78}] 70.89%; P[sp ^{1.61}]	30.07%; Mo[sp ^{2.07} d ^{1.76}] 69.93%; P[sp ^{1.59}]	31.54%; W[sp ^{2.11} d ^{1.74}] ;68.46%; P[sp ^{1.57}]
N-H	σ	70.28%; N[sp ^{4.35}] 9.72%; H[s]	70.65%; N[sp ^{4.63}] 29.35%; H[s]	70.85%; N[sp ^{4.80}] 29.15%; H[s]
N-M	σ	13.37%; Cr[sp ^{3.53} d ^{4.22}] 86.63%; N[sp ^{2.64}]	13.19%; Mo[sp ^{5.51} d ^{5.16}] 86.81%; N[sp ^{2.38}]	13.92%; W[sp ^{5.99} d ^{5.26}] 86.08%; N[sp ^{2.19}]
M-NO	σ	22.48%; Cr[sp ^{2.12} d ^{1.75}] 77.52%; N[sp ^{0.47}]	21.44%; Mo[sp ^{2.12} d ^{1.97}] 78.56%; N[sp ^{0.48}]	22.18%; W[sp ^{2.06} d ^{2.08}] 77.82%; N[sp ^{0.47}]
	π	51.04%; Cr[pd ^{9.04}] 48.96%; N[p]	49.39%; Mo[pd ^{13.01}] 50.61%; N[p]	46.03%; W[pd ^{14.02}] 53.97%; N[p]
	π	52.47%; Cr[pd ^{9.53}] 47.53%; N[p]	49.74%; Mo[pd ^{13.32}] 50.26%; N[p]	45.95%; W[pd ^{15.05}] 54.05%; N[p]

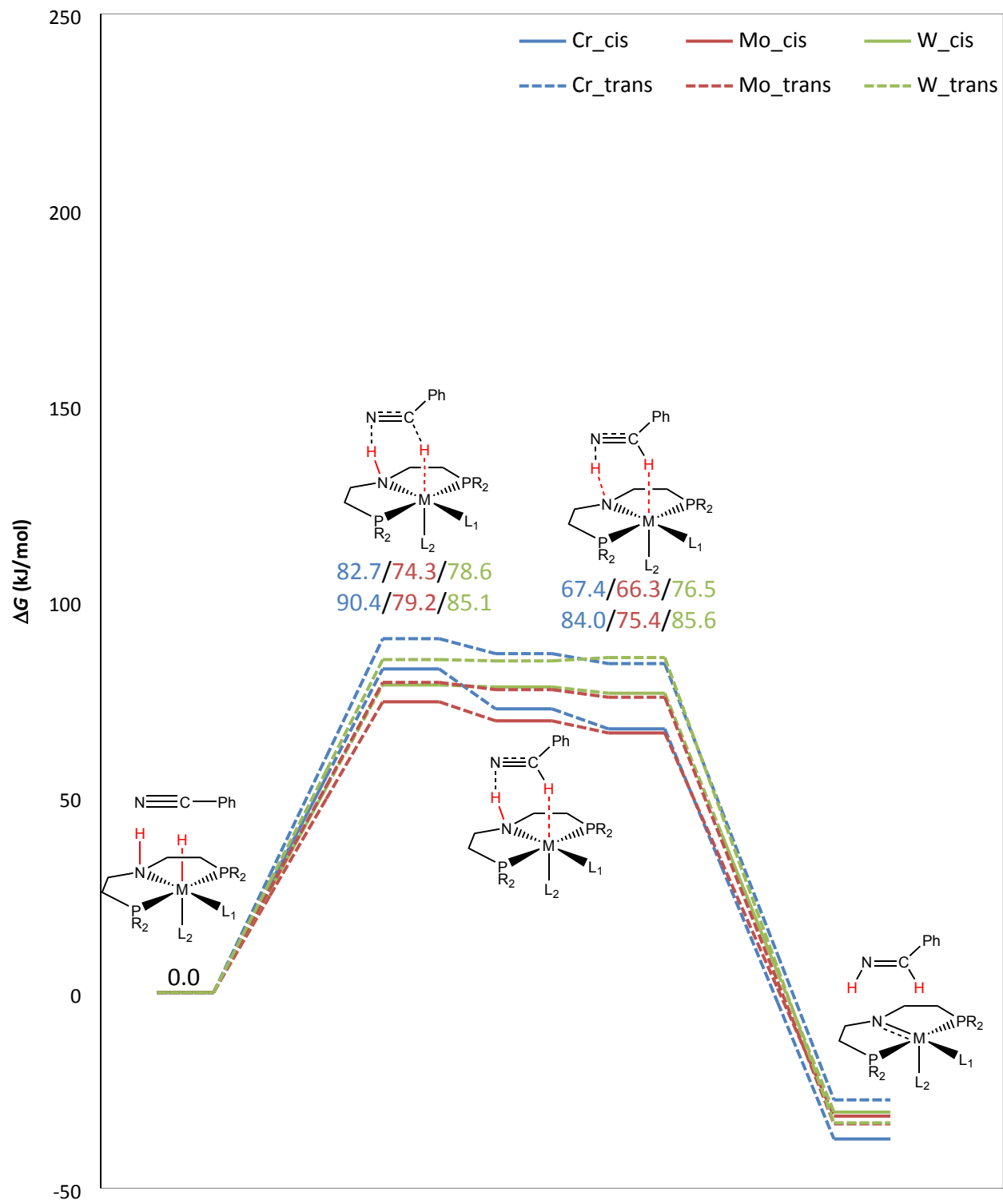
Table S6. Wiberg bonding indexes (WBI) of M-PNP (**1**) and H-M-PN^HP (**2**).

	1Cr-cis	2Cr-cis	1Mo-cis	2Mo-cis	1W-cis	2W-cis
M-N	0.874	0.375	1.223	0.389	0.915	0.417
M-P	0.677	0.727	0.720	0.769	0.780	0.831
M-L ₁	1.747	1.750	1.770	1.798	1.812	1.836
M-L ₂	1.184	1.202	1.319	1.274	1.405	1.382
M-H	--	0.699	--	0.755	--	0.790
N-H	--	0.789	--	0.785	--	0.783
	1Cr-trans	2Cr-trans	1Mo-trans	2Mo-trans	1W-trans	2W-trans
M-N	0.855	0.380	1.229	0.392	0.907	0.426
M-P	0.677	0.724	0.722	0.769	0.782	0.832
M-L ₁	1.235	1.194	1.346	1.278	1.423	1.363
M-L ₂	1.703	1.755	1.746	1.792	1.797	1.846
M-H	--	0.685	--	0.757	--	0.791
N-H	--	0.795	--	0.789	--	0.786

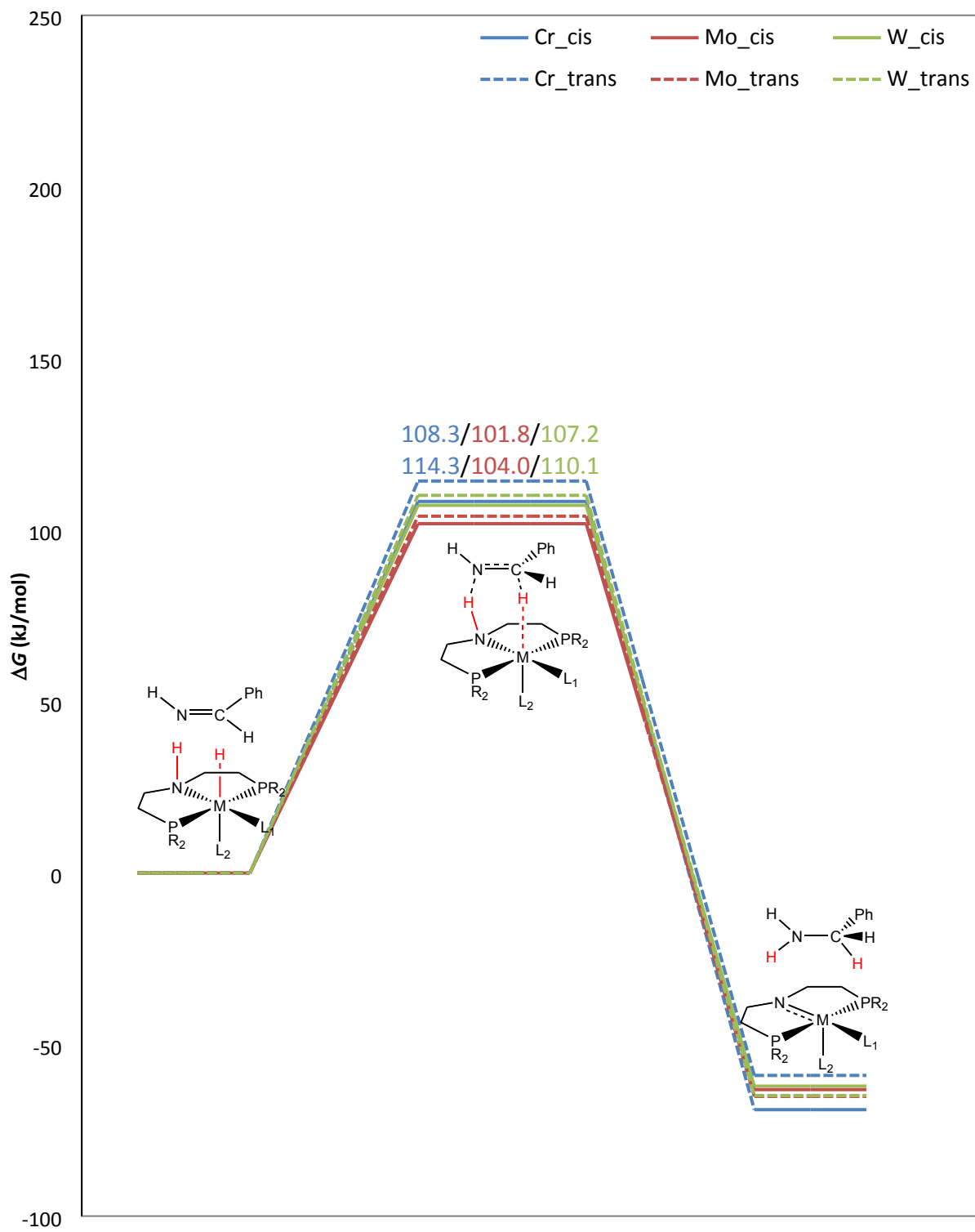
Scheme S1. Potential energy surface for M-PNP and H-M-PN^HP interconversion



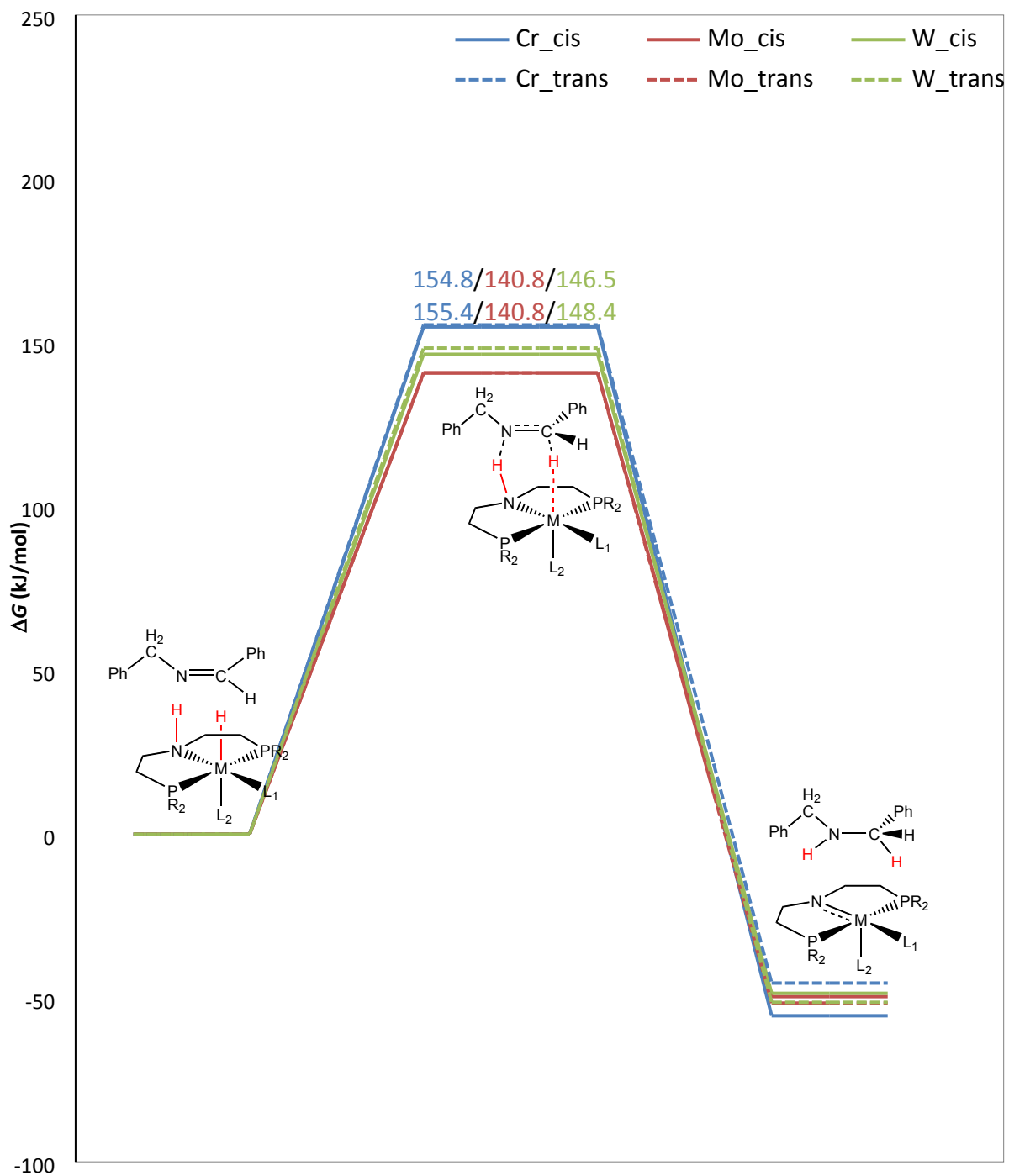
Scheme S2. Potential energy surface of benzonitrile hydrogenation



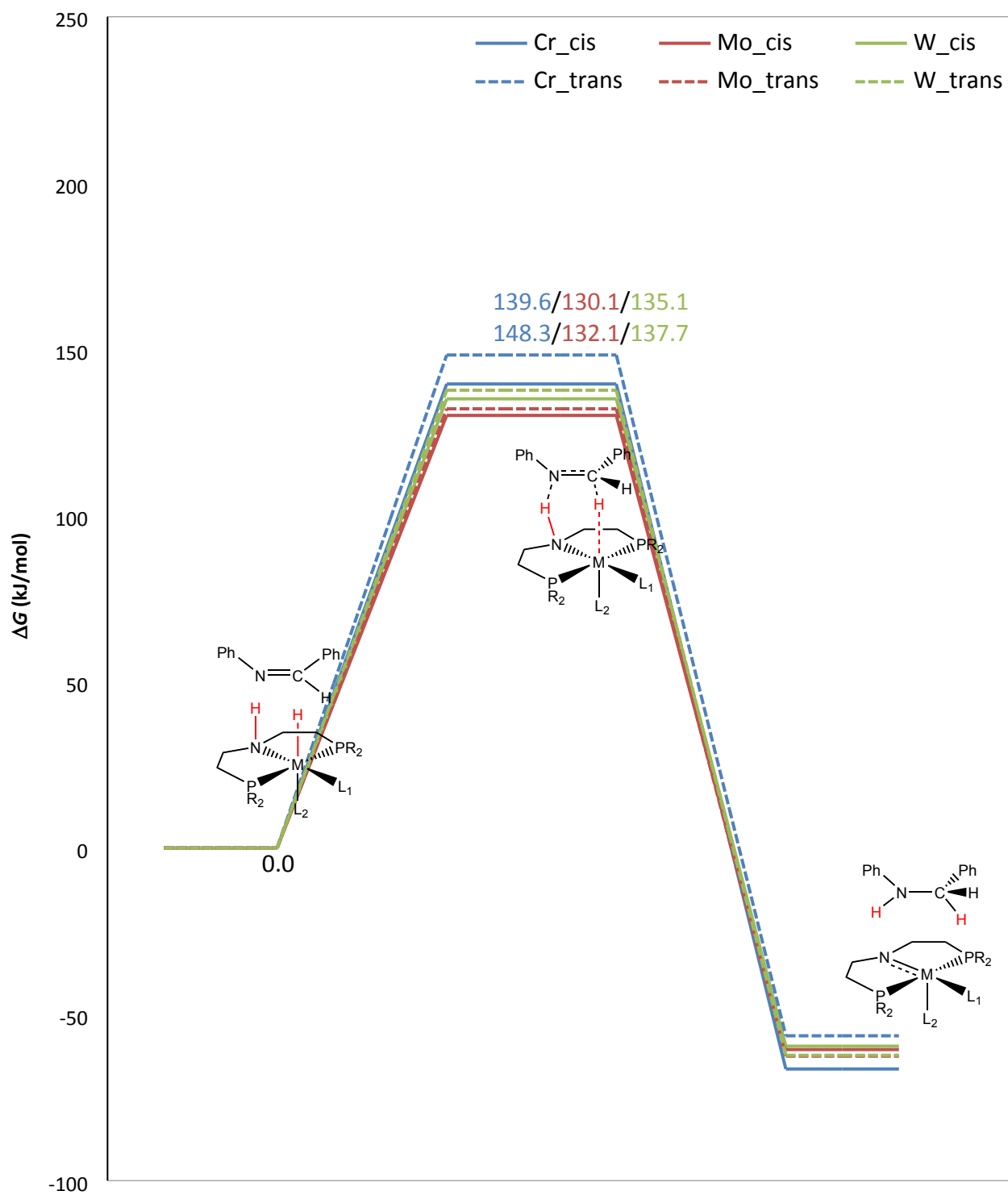
Scheme S3. Potential energy surface of phenylmethanimine hydrogenation



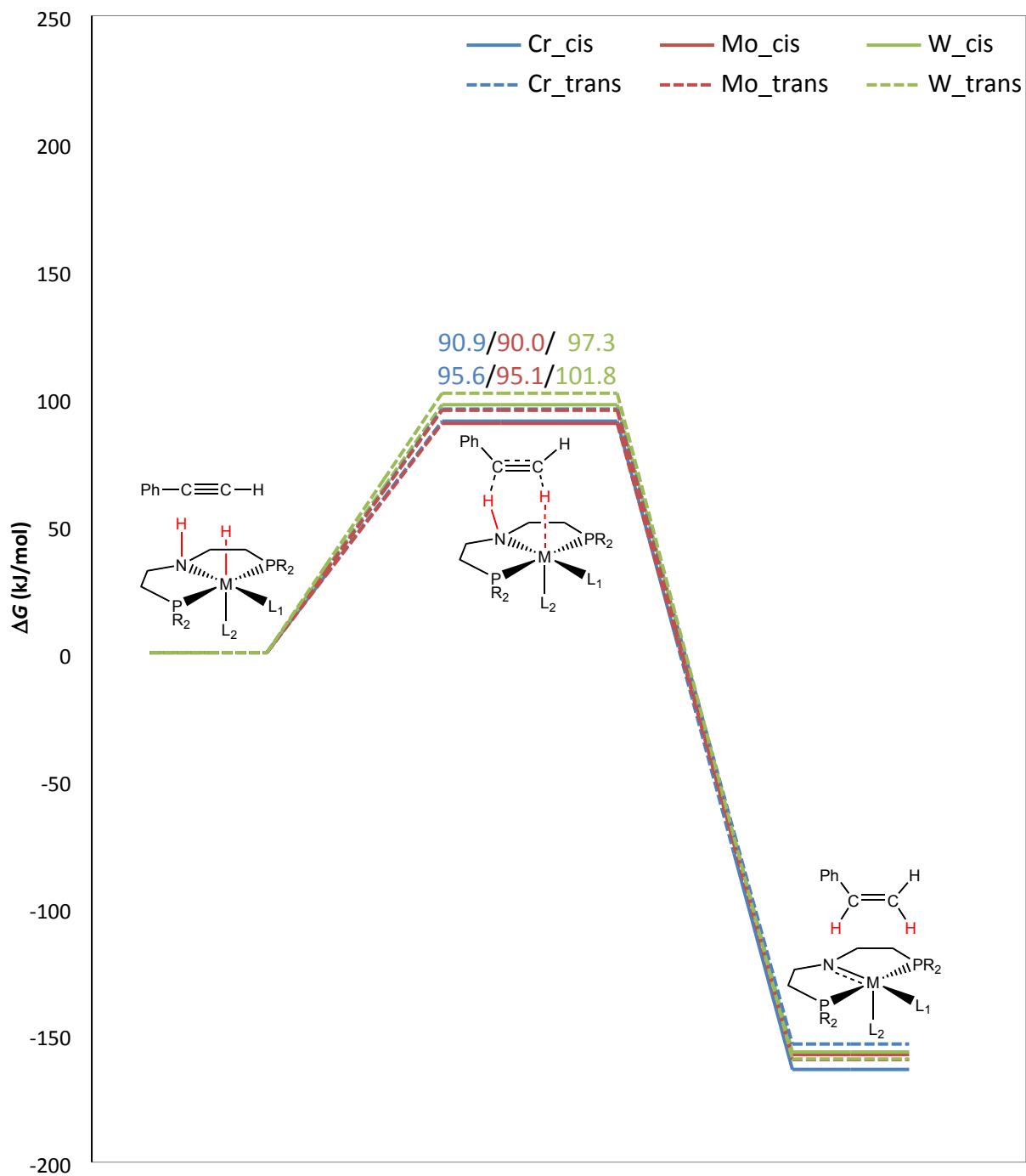
Scheme S4. Potential energy surface of Ph-CH=N-CH₂-Ph hydrogenation



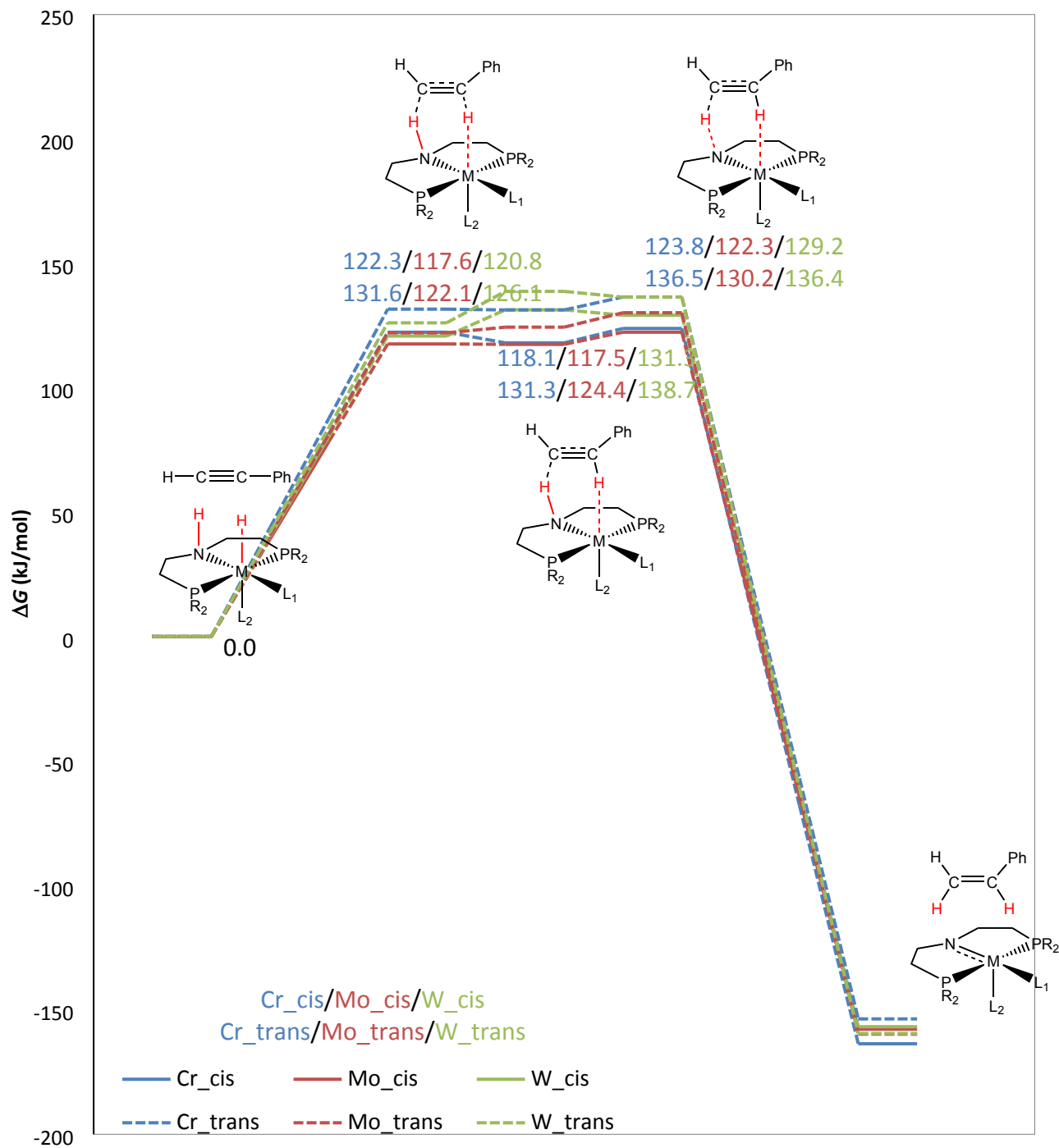
Scheme S5. Potential energy surface of Ph-CH=N-Ph hydrogenation



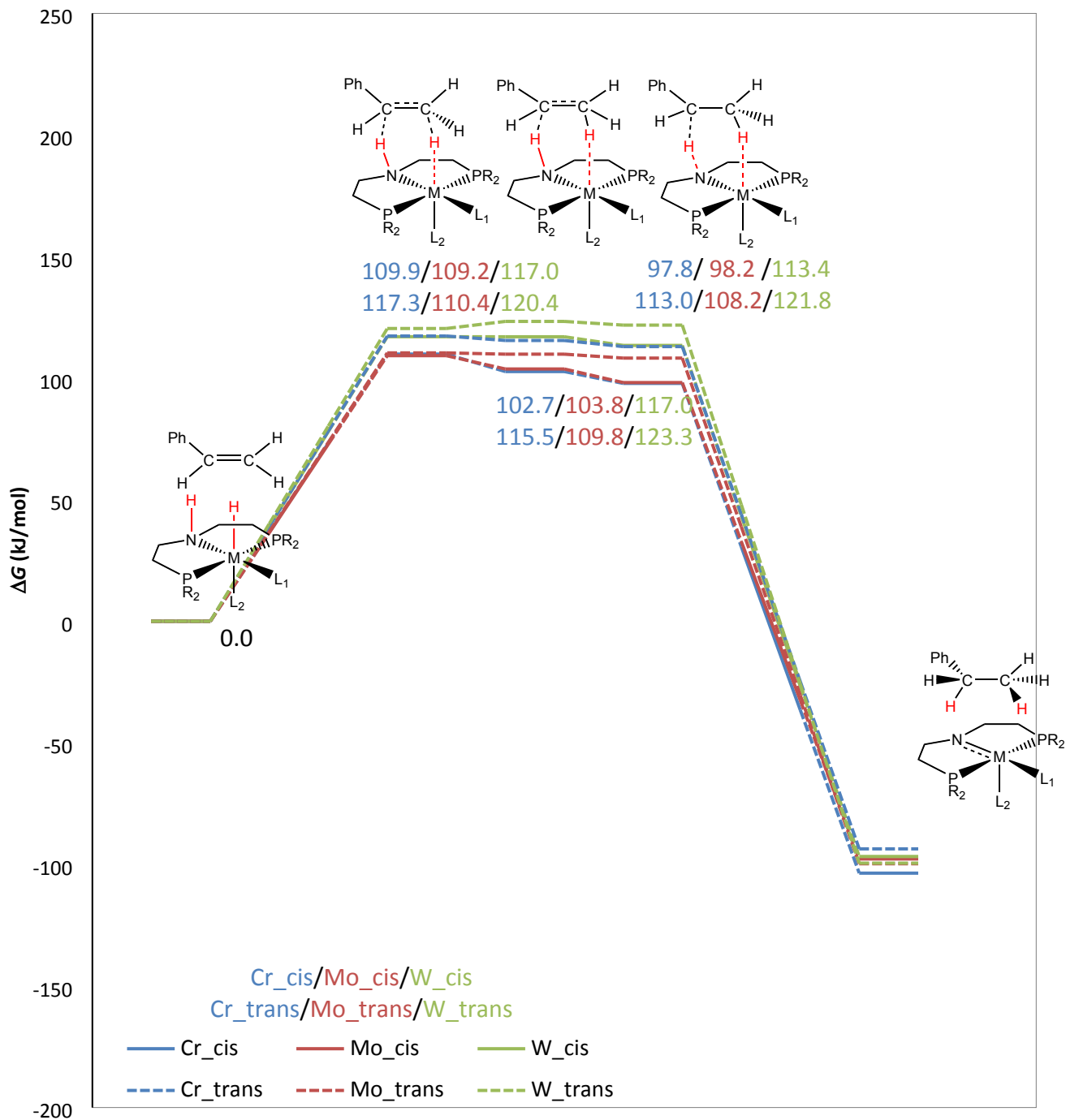
Scheme S6. Potential energy surface of phenylacetylene hydrogenation (H_M transfer to $C-H$)



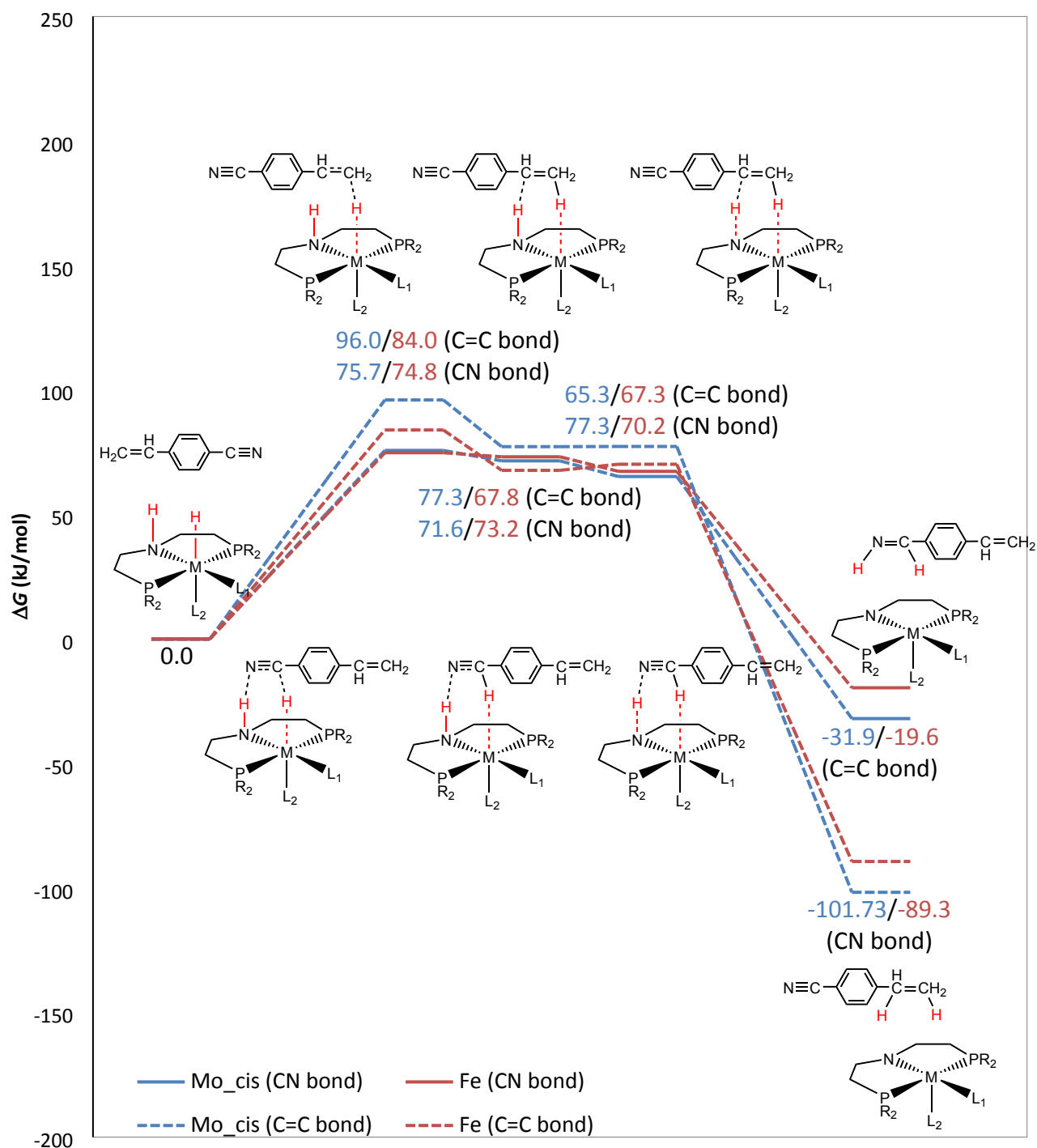
Scheme S7. Potential energy surface of phenylacetylene hydrogenation (H_M transfer to Ph-C)



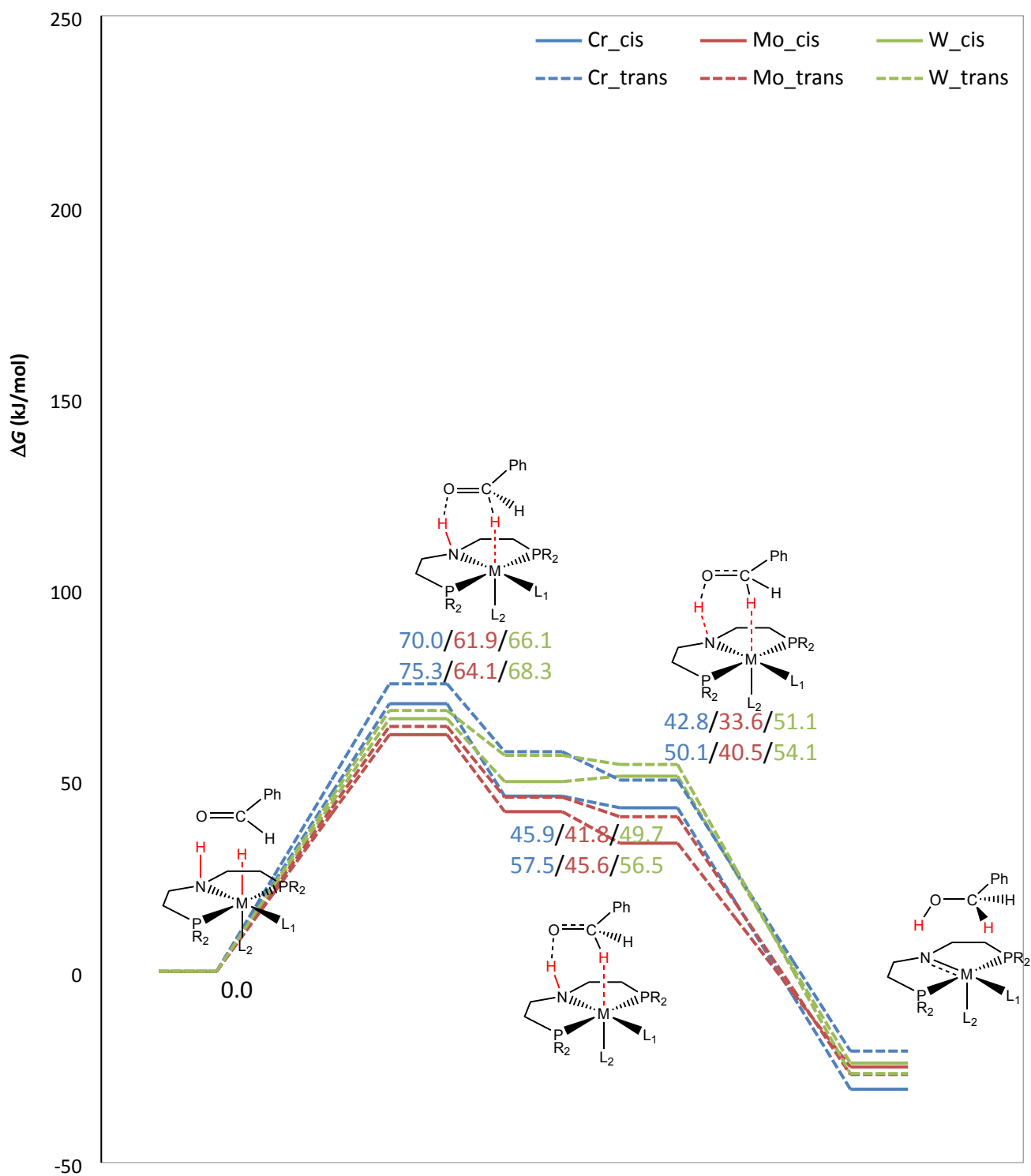
Scheme S8. Potential energy surface of styrene hydrogenation



Scheme S9. Potential energy surface of 4-vinylbenzotrile hydrogenation



Scheme S10. Potential energy surface of benzaldehyde hydrogenation



Scheme S11. Potential energy surface of acetophenone hydrogenation

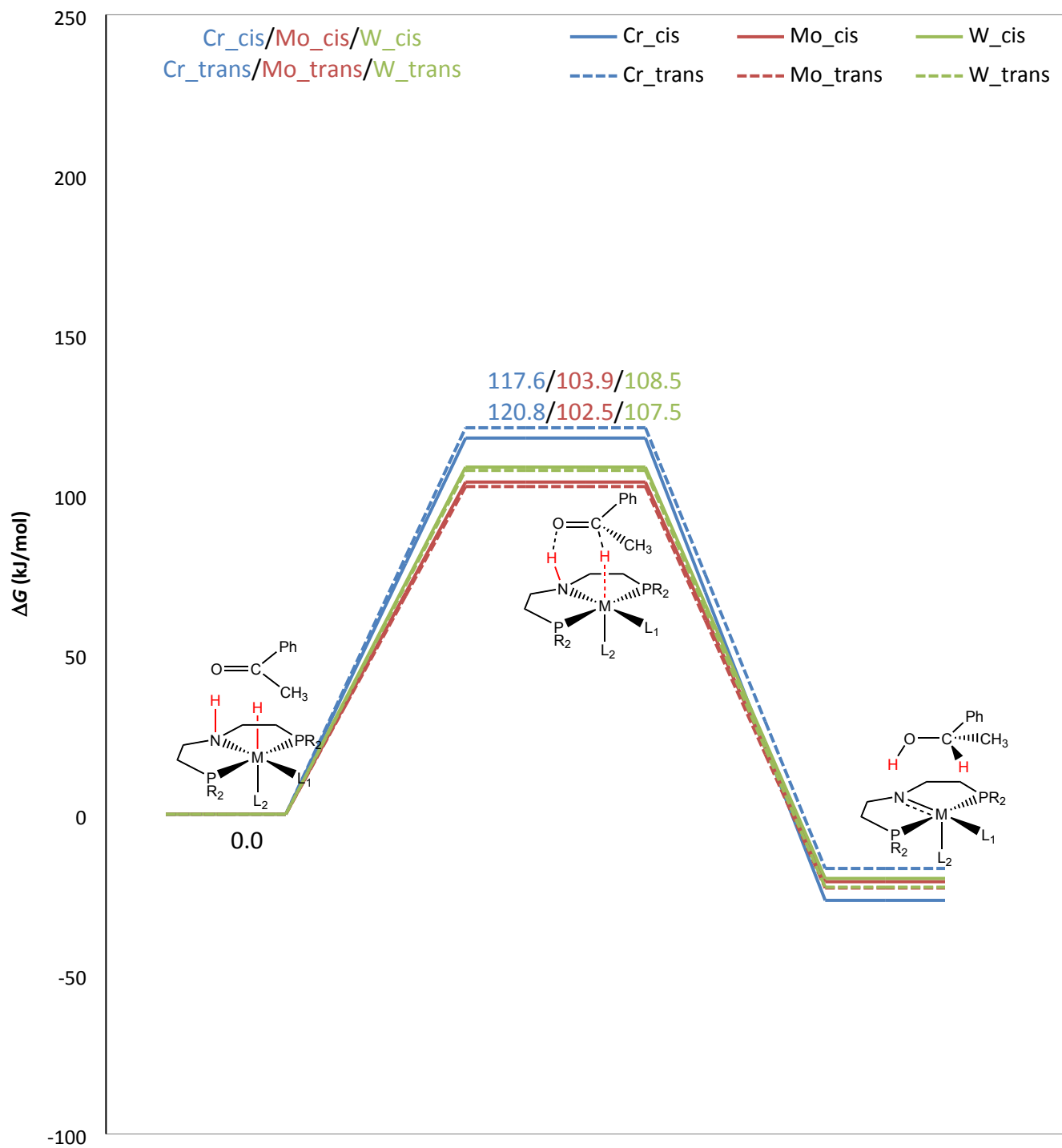


Table S7. Optimized Cartesian Coordinates

<p>H₂</p> <p>H 0.00000000 0.00000000 0.37255500 H 0.00000000 0.00000000 -0.37255500</p>	<p>Ph-C≡N</p> <p>C -0.60749500 0.00033600 0.00000400 C 0.09003600 -1.21136200 0.00002700 C 1.47583300 -1.20504300 0.00003700 C 2.16954600 -0.00032600 0.00003200 C 0.09054200 1.21164900 -0.00001300 C 1.47637700 1.20466200 0.00000800 H -0.45907500 -2.14500800 0.00002800 H 2.01657100 -2.14429100 0.00003300 H 3.25361100 -0.00056900 0.00003400 H -0.45810200 2.14557100 -0.00005500 H 2.01750100 2.14368500 0.00000700 C -2.03543700 0.00055900 -0.00003100 N -3.18955900 -0.00032000 -0.00006200</p>
<p>Ph-CH=NH</p> <p>N -1.48633800 2.45239400 0.00000000 C -0.29934900 1.99993000 0.00000000 C 0.00000000 0.56097900 0.00000000 C 1.32840000 0.13547800 0.00000000 C 1.63527000 -1.21890600 0.00000000 C 0.61281900 -2.15844200 0.00000000 C -1.02326600 -0.39138800 0.00000000 C -0.71645300 -1.74108700 0.00000000 H 2.12598800 0.87252200 0.00000000 H 2.67066800 -1.54051000 0.00000000 H 0.84880300 -3.21689900 0.00000000 H -2.05050700 -0.04633200 0.00000000 H -1.51358600 -2.47634600 0.00000000 H 0.58655000 2.65029500 0.00000000 H -1.48806500 3.47113900 0.00000000</p>	<p>Ph-CH₂NH₂</p> <p>N 1.82388100 2.18399800 0.00000000 C 0.41156000 1.95635900 0.00000000 C 0.00000000 0.50176500 0.00000000 C -1.36708700 0.21011300 0.00000000 C -1.82437700 -1.09732400 0.00000000 C -0.91836300 -2.15355400 0.00000000 C 0.89455400 -0.56301700 0.00000000 C 0.43989800 -1.87951000 0.00000000 H -2.08260600 1.02741900 0.00000000 H -2.89081800 -1.29492400 0.00000000 H -1.27128400 -3.17864700 0.00000000 H 1.96481800 -0.39416400 0.00000000 H 1.15839300 -2.69199600 0.00000000 H -0.06462900 2.42077100 0.87799300 H 2.18197900 3.11743400 0.00000000 H -0.06462900 2.42077100 -0.87799300 H 2.48449500 1.43636400 0.00000000</p>
<p>Ph-CH=NCH₂-Ph</p> <p>C -3.82426600 1.51515500 0.18137100 C -2.57639600 0.96228000 0.41238100 C -2.31890600 -0.36555800 0.05905500 C -3.33515900 -1.12240000 -0.52592900 C -4.58655300 -0.56698900 -0.75721100 C -4.83295300 0.75298700 -0.40374000 H -4.01728500 2.54587700 0.45774600 H -1.78172600 1.54123100 0.86737600 H -3.14054200 -2.15432700 -0.80202200 H -5.36854200 -1.16394900 -1.21288900 H -5.80909700 1.19005300 -0.58268100 C -1.00687900 -0.98251200 0.28865300 N -0.02632800 -0.36607700 0.79970800 H -0.92366500 -2.03803000 -0.01731200 C 1.21033800 -1.09188100 0.98403600 H 1.38224700 -1.16727000 2.06618900 H 1.15300400 -2.12124600 0.59718000 C 2.39590400 -0.38763300 0.36298100 C 3.42867200 -1.13135800 -0.20253500 C 2.49748800 1.00237400 0.37491100 C 4.54695700 -0.50324700 -0.73767900 H 3.35759000 -2.21462300 -0.22820200 C 3.61203900 1.63156600 -0.16317700</p>	<p>Ph-CH₂NHCH₂-Ph</p> <p>C -3.61290100 1.51458600 0.30367300 C -2.33572200 0.97242600 0.33146100 C -2.09265300 -0.30201800 -0.18277400 C -3.15900900 -1.01847300 -0.72121000 C -4.43870000 -0.47603700 -0.75502400 C -4.66924100 0.79320700 -0.24233900 H -3.78570700 2.50669000 0.70682800 H -1.51228700 1.53019200 0.76256400 H -2.98606600 -2.01421500 -1.11813800 H -5.25647400 -1.04910100 -1.17834400 H -5.66674600 1.21797000 -0.26423900 C -0.70218600 -0.88271200 -0.17561000 N -0.05519100 -0.73673600 1.12078200 H -0.75015000 -1.93432700 -0.50700500 C 1.28238400 -1.30516600 1.17562700 H 1.56408900 -1.37391600 2.23196900 H 1.32622100 -2.33135700 0.77144400 C 2.31027400 -0.46276100 0.45476700 C 3.26748800 -1.05471100 -0.36484800 C 2.34121700 0.92050700 0.62941300 C 4.24059400 -0.28638100 -0.99406800 H 3.24878800 -2.12986900 -0.51665200 C 3.30819700 1.69112200 -0.00058700</p>

H 1.68919000 1.58524800 0.79986100 C 4.64212100 0.88191200 -0.71937400 H 5.34118900 -1.09806200 -1.17556800 H 3.67628800 2.71430400 -0.14968000 H 5.51120400 1.37514900 -1.14039900	H 1.58819200 1.38449000 1.25657100 C 4.26382800 1.08980900 -0.81292100 H 4.97722600 -0.76403600 -1.63093500 H 3.31919900 2.76619200 0.14373200 H 5.01894800 1.69250400 -1.30533400 H -0.08267100 -0.35832300 -0.91240300 H -0.63764400 -1.14613200 1.84111100
Ph-CH=N-Ph C -1.84020900 -0.17298500 0.08590900 C -2.70782800 -1.20193400 0.45927000 C -2.37405300 1.03804200 -0.36762300 C -4.08281500 -1.02852700 0.38315900 H -2.29826800 -2.14361300 0.81189800 C -3.74525100 1.20943600 -0.44163900 H -1.69208800 1.82932100 -0.65529200 C -4.60355200 0.17775600 -0.06698900 H -4.74766800 -1.83336900 0.67573600 H -4.15318900 2.15060800 -0.79333600 H -5.67732100 0.31645900 -0.12758800 C -0.39577800 -0.38749000 0.17550700 H -0.08382600 -1.37908100 0.53302200 N 0.45566100 0.51070700 -0.12049900 C 1.82442000 0.22258700 -0.07055200 C 2.36671300 -0.98261000 -0.53090900 C 2.68601900 1.21186600 0.41297300 C 3.73643500 -1.19966700 -0.47585400 H 1.71474500 -1.73266900 -0.96483500 C 4.05030900 0.98022700 0.48346300 H 2.26006300 2.15265200 0.74147800 C 4.58305600 -0.22573800 0.03897500 H 4.14543100 -2.13321100 -0.84694600 H 4.70525500 1.75056600 0.87558400 H 5.65244400 -0.39839500 0.07961900	Ph-CH₂NH-Ph C 1.88822700 0.37586200 -0.12181200 C 2.74092200 0.98339800 0.79568900 C 2.39045800 -0.64137400 -0.93499700 C 4.07100400 0.59046400 0.89806000 H 2.36081200 1.77299000 1.43624200 C 3.71591000 -1.03843100 -0.83201500 H 1.73186000 -1.12318600 -1.65003200 C 4.56106100 -0.42164700 0.08460600 H 4.72262800 1.07497000 1.61680400 H 4.09368100 -1.82797000 -1.47237400 H 5.59747600 -0.73047800 0.16322900 C 0.44769800 0.80236600 -0.23722200 H 0.25151800 1.13472700 -1.26327800 H 0.26928000 1.66987100 0.41554500 N -0.44066500 -0.29991200 0.07032900 H -0.08071400 -0.94226200 0.75872100 C -1.81722100 -0.16036900 0.06392300 C -2.61566100 -1.17249000 0.62110100 C -2.45665100 0.94418700 -0.51332800 C -3.99518300 -1.08203800 0.59431100 H -2.13778000 -2.03755300 1.07106700 C -3.84414700 1.01835200 -0.53885500 H -1.87501700 1.74989000 -0.94326600 C -4.62644700 0.01374500 0.01122100 H -4.58645700 -1.87845500 1.03355800 H -4.31489900 1.88355700 -0.99359200 H -5.70754900 0.08113300 -0.00902300
Ph-C≡CH C 1.20756500 -0.11893900 0.00000000 C 1.20337600 -1.50521100 0.00000000 C 0.00098200 -2.20244700 0.00000000 C -1.20740000 -0.11991300 0.00000000 C -1.20219000 -1.50587000 0.00000000 H 2.14282100 0.42781700 0.00000000 H 2.14413000 -2.04422200 0.00000000 H 0.00109900 -3.28662700 0.00000000 H -2.14275900 0.42666400 0.00000000 H -2.14230300 -2.04599900 0.00000000 C 0.00000000 0.59071200 0.00000000 C -0.00101500 2.01524300 0.00000000 C -0.00147400 3.21959700 0.00000000 H -0.00204600 4.28333700 0.00000000	Ph-CH=CH₂ C -1.77279800 -1.04120100 0.00001700 C -0.40472700 -1.27548200 -0.00000400 C 0.51257000 -0.21944000 -0.00001600 C 0.00911000 1.08711900 -0.00002600 C -1.35555000 1.32319000 -0.00001200 C -2.25459700 0.26064200 0.00002000 H -2.46303900 -1.87758500 0.00003800 H -0.03413100 -2.29578000 -0.00000300 H 0.69156300 1.92924100 -0.00005400 H -1.72356900 2.34341800 -0.00001500 H -3.32226000 0.44927200 0.00003300 C 1.94658200 -0.52730900 -0.00002700 H 2.17846900 -1.59044000 -0.00009200 C 2.96320600 0.33418800 0.00004000 H 2.82251200 1.40940700 0.00011700 H 3.98768000 -0.01777800 0.00002400
Ph-CH₂CH₃ C -1.90813500 -0.99847500 0.00000000 C -1.38090400 0.28369500 0.00000000 C 0.00000000 0.50089500 0.00000000 C 0.83585200 -0.61318800 0.00000000 C 0.31171100 -1.90260000 0.00000000 C -1.06066700 -2.10163000 0.00000000	Ph-CH=O C -0.28638900 2.01845100 0.00000000 C 0.00000000 0.56986600 0.00000000 C 1.32413400 0.13334600 0.00000000 C 1.61131700 -1.22442400 0.00000000 C 0.57231500 -2.14728100 0.00000000 C -1.04034100 -0.36211000 0.00000000

H -2.98371700 -1.13907800 0.00000000	C -0.75278000 -1.71605600 0.00000000
H -2.05199500 1.13789800 0.00000000	H 2.12805000 0.86360000 0.00000000
H 1.91161500 -0.48294600 0.00000000	H 2.64069300 -1.56422600 0.00000000
H 0.98406600 -2.75386000 0.00000000	H 0.79404200 -3.20885300 0.00000000
H -1.46920300 -3.10600100 0.00000000	H -2.06251500 -0.00097200 0.00000000
C 0.52153300 1.92052900 0.00000000	H -1.55771000 -2.44235900 0.00000000
H 0.10409600 2.43810100 0.87141800	O -1.39111800 2.50699000 0.00000000
H 0.10409600 2.43810100 -0.87141800	H 0.61684900 2.66613300 0.00000000
C 2.03414300 2.08640500 0.00000000	
H 2.49069200 1.63394400 -0.88385400	
H 2.29846200 3.14610400 0.00000000	
H 2.49069200 1.63394400 0.88385400	
Ph-CH₂OH	Ph-CO-CH₃
O 1.89155300 1.98666800 0.00000000	C 0.26225100 1.68526600 0.00000000
C 0.47652200 1.93999900 0.00000000	C 0.00000000 0.21189500 0.00000000
H 0.06891700 2.44954500 0.88520800	C 1.02711000 -0.73382800 0.00000000
C 0.00000000 0.51167900 0.00000000	C 0.73357800 -2.09080800 0.00000000
C 0.89131800 -0.55550800 0.00000000	C -0.58918000 -2.51516300 0.00000000
C 0.41892300 -1.86375900 0.00000000	C -1.32662200 -0.22622500 0.00000000
C -0.94524800 -2.11903500 0.00000000	C -1.61944800 -1.57969000 0.00000000
C -1.36992400 0.24962100 0.00000000	H 2.06318600 -0.41656000 0.00000000
C -1.84084900 -1.05504500 0.00000000	H 1.53793800 -2.81775600 0.00000000
H 1.95455900 -0.35252800 0.00000000	H -0.81823600 -3.57515200 0.00000000
H 1.12462800 -2.68749200 0.00000000	H -2.11312400 0.51918200 0.00000000
H -1.31091100 -3.13983500 0.00000000	H -2.65217800 -1.91012400 0.00000000
H -2.07707600 1.07452900 0.00000000	O -0.65773900 2.47735400 0.00000000
H -2.90906000 -1.24267300 0.00000000	C 1.69377800 2.16789600 0.00000000
H 0.06891700 2.44954500 -0.88520800	H 2.22969100 1.80485700 0.88110400
H 2.16315800 2.90785400 0.00000000	H 2.22969100 1.80485700 -0.88110400
	H 1.69613900 3.25581300 0.00000000
Ph-CH(OH)-CH₃	1Cr-cis-Cs
H 1.83460600 -1.28024200 -0.77868900	O -2.85592400 1.07381700 0.00000000
H 1.86351900 0.85028600 -1.75572000	N -1.77975400 0.58466700 0.00000000
C 1.65020600 -0.34564300 -0.22923700	Cr -0.18751600 0.12685900 0.00000000
C 0.15036700 -0.15452400 -0.13286400	P 0.12813400 0.23347500 -2.31876900
C -0.71205100 -1.23483700 -0.30388600	P 0.12813400 0.23347500 2.31876900
C -2.08667400 -1.07469900 -0.17765900	C 1.13402100 1.78084300 -2.45088300
C -2.61638600 0.17476300 0.11763700	C 1.13402100 1.78084300 2.45088300
C -0.39080400 1.09639600 0.16323200	H 0.41056700 2.59790500 -2.52156800
C -1.76410300 1.26058800 0.28400300	H 0.41056700 2.59790500 2.52156800
H -0.30350100 -2.21197000 -0.54478000	H 1.76387300 1.81145200 -3.34411300
H -2.74466900 -1.92559000 -0.31662000	H 1.76387300 1.81145200 3.34411300
H -3.68886900 0.30386400 0.21191200	C 1.95035200 1.93805400 -1.17680800
H 0.27395900 1.94460100 0.28532700	C 1.95035200 1.93805400 1.17680800
H -2.17173100 2.23974800 0.51116600	H 2.15887200 3.00897300 -1.02675100
O 2.28942600 0.73721000 -0.89999800	H 2.15887200 3.00897300 1.02675100
C 2.30517000 -0.45329400 1.13783000	H 2.93936500 1.46786100 -1.29989400
H 1.88498800 -1.28892300 1.70028500	H 2.93936500 1.46786100 1.29989400
H 3.38033500 -0.60632600 1.02617600	N 1.27317700 1.39638600 0.00000000
H 2.14161200 0.46437300 1.70658900	C -1.35474700 0.62728300 3.40057500
	C -1.35474700 0.62728300 -3.40057500
	H -1.68935500 1.56940200 2.95022200
	H -1.68935500 1.56940200 -2.95022200
	C 1.15507000 -1.03328100 3.25575700
	C 1.15507000 -1.03328100 -3.25575700
	C 2.47722600 -1.27605600 2.52924100
	C 2.47722600 -1.27605600 -2.52924100
	C -0.57171200 -1.67455400 0.00000000
	O -0.83241400 -2.80281900 0.00000000
	H 1.37312700 -0.57513100 -4.22722100

	H 1.37312700 -0.57513100 4.22722100 C 0.42339600 -2.35268700 -3.48992900 C 0.42339600 -2.35268700 3.48992900 H -0.44912500 -2.23626800 -4.13292900 H -0.44912500 -2.23626800 4.13292900 H 0.09420100 -2.80511200 -2.55284900 H 0.09420100 -2.80511200 2.55284900 H 1.09722200 -3.06190000 -3.98050800 H 1.09722200 -3.06190000 3.98050800 C -2.50403400 -0.36884200 3.25731100 C -2.50403400 -0.36884200 -3.25731100 H -2.28990800 -1.31658800 3.75373900 H -2.28990800 -1.31658800 -3.75373900 H -2.73093400 -0.57722900 2.21242200 H -2.73093400 -0.57722900 -2.21242200 H -3.40548100 0.04407700 3.71952400 H -3.40548100 0.04407700 -3.71952400 C -1.00842600 0.88956100 4.86410100 C -1.00842600 0.88956100 -4.86410100 H -0.22027700 1.63724200 4.97835600 H -0.22027700 1.63724200 -4.97835600 H -0.68482100 -0.02307500 5.37090200 H -0.68482100 -0.02307500 -5.37090200 H -1.89064000 1.25855700 5.39607000 H -1.89064000 1.25855700 -5.39607000 H 3.07403300 -2.00893300 3.08050100 H 2.30752400 -1.67097000 1.52479800 H 3.07429900 -0.36795700 2.43633000 H 3.07403300 -2.00893300 -3.08050100 H 3.07429900 -0.36795700 -2.43633000 H 2.30752400 -1.67097000 -1.52479800
1Cr-trans-Cs	1Cr-C1
O 1.13237700 2.59188200 0.00000000 N 0.76310700 1.46854900 0.00000000 Cr 0.16125200 -0.09109100 0.00000000 P -0.12636200 -0.22142300 -2.31689700 P -0.12636200 -0.22142300 2.31689700 C -1.12764600 -1.77053500 -2.45393600 C -1.12764600 -1.77053500 2.45393600 H -0.40329700 -2.58514600 -2.54075500 H -0.40329700 -2.58514600 2.54075500 H -1.76112500 -1.79150100 -3.34486500 H -1.76112500 -1.79150100 3.34486500 C -1.94038300 -1.94759400 -1.17829600 C -1.94038300 -1.94759400 1.17829600 H -2.13053400 -3.02304200 -1.03348000 H -2.13053400 -3.02304200 1.03348000 H -2.93722100 -1.49402200 -1.30001500 H -2.93722100 -1.49402200 1.30001500 N -1.27772000 -1.39711200 0.00000000 C 1.33463700 -0.58600500 3.43987000 C 1.33463700 -0.58600500 -3.43987000 H 1.66418000 -1.55140400 3.03736800 H 1.66418000 -1.55140400 -3.03736800 C -1.16230900 1.07329200 3.20152700 C -1.16230900 1.07329200 -3.20152700 C -2.49698800 1.25639000 2.48140700 C -2.49698800 1.25639000 -2.48140700 C 1.79064500 -0.88384100 0.00000000 O 2.80859400 -1.43580900 0.00000000 H -1.35962000 0.67399000 -4.20285100 H -1.35962000 0.67399000 4.20285100	C -2.46005800 -0.61010400 1.93692200 H -2.58814700 0.29564600 2.53335200 H -3.32381300 -1.25471100 2.11843200 C -1.15151100 -1.28538400 2.32175000 H -1.03577700 -1.22609100 3.41477600 H -1.20194800 -2.36140400 2.09043600 C 1.19299400 -1.04266100 2.43371200 H 1.40521400 -2.11867400 2.32753500 H 1.00196400 -0.88764700 3.50701800 C 2.41868200 -0.23310100 2.03584200 H 3.34844300 -0.72523200 2.33283300 H 2.38623400 0.74127100 2.52758400 C -3.31345300 1.52078100 0.07328700 H -3.19707900 1.83070500 -0.97064200 C -4.80052700 1.37261700 0.38567600 H -4.96067500 0.99428200 1.39942500 H -5.31356400 0.70552200 -0.30884300 H -5.29236000 2.34818700 0.32272100 C -2.67771000 2.60177800 0.94672900 H -3.14290700 3.56868700 0.73540000 H -1.60709000 2.69684200 0.76652400 H -2.82530600 2.39687500 2.01041700 C -3.38869100 -1.30358500 -0.76957400 H -4.37776100 -1.26895500 -0.29991100 C -3.52260000 -0.90734700 -2.23803600 H -2.54957700 -0.88511000 -2.73253300 H -3.98596900 0.07355500 -2.36366900 H -4.14611500 -1.63510100 -2.76589600 C -2.84274300 -2.72210400 -0.62371300 H -3.49186000 -3.42567700 -1.15363900

C -0.43860500	2.41160700	-3.33621100	H -2.79629700	-3.04088400	0.41968000
C -0.43860500	2.41160700	3.33621100	H -1.84202500	-2.80943600	-1.04986800
H 0.45042500	2.34257900	-3.96349900	C 3.32425800	1.64210100	-0.06244200
H 0.45042500	2.34257900	3.96349900	H 4.31091700	1.45247300	0.37451700
H -0.13378800	2.80472000	-2.36441700	C 3.48507400	1.91278200	-1.55862700
H -0.13378800	2.80472000	2.36441700	H 2.51748900	2.08894700	-2.03226000
H -1.10693200	3.14506000	-3.79780200	H 3.97387200	1.08992100	-2.08394300
H -1.10693200	3.14506000	3.79780200	H 4.09581400	2.80764600	-1.71046800
C 2.49513200	0.39153500	3.26291400	C 2.70895700	2.85012600	0.64107400
C 2.49513200	0.39153500	-3.26291400	H 3.34270300	3.72769000	0.48156100
H 2.29135300	1.35798400	3.72675100	H 2.61741000	2.70770900	1.71936300
H 2.29135300	1.35798400	-3.72675100	H 1.71954300	3.07914800	0.24324500
H 2.71923200	0.56516800	2.21025700	C 3.35234400	-1.26261000	-0.57657800
H 2.71923200	0.56516800	-2.21025700	H 3.18356800	-1.11911400	-1.64910000
H 3.39410600	-0.01378600	3.73643600	C 2.81126500	-2.64199700	-0.20039600
H 3.39410600	-0.01378600	-3.73643600	H 3.26265500	-3.40768800	-0.83745600
C 0.96945200	-0.77825700	4.90943000	H 1.72833300	-2.70338300	-0.31646200
C 0.96945200	-0.77825700	-4.90943000	H 3.05742600	-2.89206100	0.83469700
H 0.16914700	-1.50910100	5.04731200	C 4.85038400	-1.17663100	-0.29624900
H 0.16914700	-1.50910100	-5.04731200	H 5.06425400	-1.24793400	0.77406100
H 0.65354400	0.16049300	5.37131200	H 5.29848800	-0.25432200	-0.66853200
H 0.65354400	0.16049300	-5.37131200	H 5.36647700	-2.00963400	-0.78360600
H 1.84012900	-1.13550600	5.46783300	N -0.08607300	1.49278800	-1.02340600
H 1.84012900	-1.13550600	-5.46783300	N 0.00528200	-0.67687300	1.66428700
H -3.08741500	2.02812700	2.98432900	O -0.16367800	2.52088300	-1.60231100
H -2.34410500	1.57222700	1.44659200	P -2.32822500	-0.07621100	0.17108400
H -3.09208500	0.34218700	2.46947900	P 2.31434000	0.08855300	0.21970500
H -3.08741500	2.02812700	-2.98432900	Cr -0.00537200	0.09241000	-0.12077000
H -3.09208500	0.34218700	-2.46947900	C 0.10779500	-0.91734600	-1.62918400
H -2.34410500	1.57222700	-1.44659200	O 0.20535900	-1.54967200	-2.59486700
1Cr-C1-triplet			2Cr-cis-Cs		
C -2.30227505	0.45160961	1.98307961	O 2.53744900	1.75879600	0.00000000
H -2.04551874	1.49787280	2.17071847	C 1.57339000	1.10966100	0.00000000
H -3.27052303	0.24976559	2.44916254	Cr -0.00958000	0.16716500	0.00000000
C -1.18869119	-0.43396796	2.54244056	H -1.27879600	-0.90502100	0.00000000
H -1.00906635	-0.13466610	3.58917818	P -0.09216600	-0.30873100	2.26940000
H -1.55036818	-1.47899415	2.59837562	P -0.09216600	-0.30873100	-2.26940000
C 1.18047212	-0.78473736	2.46850705	C 0.90810400	-1.88826700	2.42443400
H 1.33733981	-1.87246353	2.33212813	C 0.90810400	-1.88826700	-2.42443400
H 1.06333779	-0.64246782	3.55507059	H 0.20129800	-2.72423200	2.41968300
C 2.44518497	-0.04155576	2.02452664	H 0.20129800	-2.72423200	-2.41968300
H 3.35495575	-0.58287515	2.29681997	H 1.45812500	-1.94068300	3.36581800
H 2.48695082	0.93553520	2.50984715	H 1.45812500	-1.94068300	-3.36581800
C -3.06050415	1.84540203	-0.53420671	C 1.85047800	-2.00911700	1.23638600
H -3.35734615	1.58227087	-1.55482029	C 1.85047800	-2.00911700	-1.23638600
C -4.28997296	2.34380054	0.22199963	H 2.32490700	-3.00128800	1.22044300
H -4.03543897	2.64118175	1.24231912	H 2.32490700	-3.00128800	-1.22044300
H -5.08489855	1.59752993	0.27769184	H 2.64510900	-1.26153900	1.29304700
H -4.70454533	3.22358875	-0.27950709	H 2.64510900	-1.26153900	-1.29304700
C -1.98789656	2.92552870	-0.62637244	N 1.09766900	-1.76868000	0.00000000
H -2.39849966	3.82732015	-1.09032222	H 0.28119300	-2.37393200	0.00000000
H -1.14020869	2.58871444	-1.22479050	C -1.74492400	-0.87478800	-2.97512700
H -1.61613221	3.20554534	0.36302470	C -1.74492400	-0.87478800	2.97512700
C -3.70964714	-0.98053027	-0.22733905	H -1.91932100	-1.76802500	-2.36392400
H -4.64924070	-0.47928682	0.02975196	H -1.91932100	-1.76802500	2.36392400
C -3.72330914	-1.31740412	-1.71786300	C 0.64302600	0.80361100	-3.59943800
H -2.78899858	-1.79418787	-2.02202751	C 0.64302600	0.80361100	3.59943800
H -3.86123408	-0.43594436	-2.34709886	C 2.16330600	0.90033900	-3.49529200
H -4.54239167	-2.00855561	-1.93746062	C 2.16330600	0.90033900	3.49529200
C -3.60210630	-2.24609688	0.61858771	N -0.94272800	1.53869000	0.00000000
H -4.41586713	-2.93087208	0.36184402	O -1.60865000	2.51111800	0.00000000
H -3.66980769	-2.03837913	1.68759479	H 0.39373100	0.34404100	4.56183100

H	-2.66252801	-2.77159849	0.43688744	H	0.39373100	0.34404100	-4.56183100
C	2.84950424	2.02824429	-0.04911501	C	0.01752900	2.19596900	3.53335200
H	3.79225413	2.16785891	0.49159978	C	0.01752900	2.19596900	-3.53335200
C	3.06488002	2.33787754	-1.52936411	H	-1.05965700	2.18028500	3.70317500
H	2.16482025	2.12337375	-2.11100113	H	-1.05965700	2.18028500	-3.70317500
H	3.88682913	1.76478686	-1.96258764	H	0.19252100	2.65458100	2.55777200
H	3.30112963	3.39826135	-1.65809957	H	0.19252100	2.65458100	-2.55777200
C	1.79941849	2.95747098	0.55113623	H	0.46310800	2.84312300	4.29501000
H	2.12834831	3.99733288	0.46241681	H	0.46310800	2.84312300	-4.29501000
H	1.60951763	2.75196570	1.60586677	C	-2.88059500	0.09612800	-2.66667700
H	0.85029677	2.85473359	0.02334960	C	-2.88059500	0.09612800	2.66667700
C	3.79489764	-0.72098210	-0.53679590	H	-2.80918300	1.01318200	-3.25525600
H	3.71507228	-0.53397001	-1.61287319	H	-2.80918300	1.01318200	3.25525600
C	3.60418659	-2.21895898	-0.31104235	H	-2.88521100	0.36504300	-1.61040400
H	4.40844201	-2.77737248	-0.79870067	H	-2.88521100	0.36504300	1.61040400
H	2.65790423	-2.57090389	-0.72218870	H	-3.84178900	-0.36889900	-2.90690300
H	3.62749034	-2.47395722	0.75202909	H	-3.84178900	-0.36889900	2.90690300
C	5.17019458	-0.26263941	-0.05832008	C	-1.72527300	-1.27932600	-4.44615600
H	5.28688343	-0.39821975	1.02027176	C	-1.72527300	-1.27932600	4.44615600
H	5.36711495	0.78575088	-0.28816343	H	-0.91616100	-1.97572000	-4.68158200
H	5.95034331	-0.85571190	-0.54564348	H	-0.91616100	-1.97572000	4.68158200
N	0.01788904	-0.18829299	-1.99869439	H	-1.62355000	-0.41093700	-5.10187800
N	0.01963938	-0.28685738	1.76612724	H	-1.62355000	-0.41093700	5.10187800
O	0.02247654	-0.02376486	-3.17938233	H	-2.66714800	-1.77023700	-4.71039200
P	-2.33926347	0.24942718	0.14395309	H	-2.66714800	-1.77023700	4.71039200
P	2.35269186	0.23735535	0.19171891	H	2.54345700	1.53753900	-4.29972000
Cr	0.00249221	-0.43055682	-0.25290208	H	2.47233800	1.34661300	-2.54944800
C	-0.04667200	-2.47531646	-0.54965163	H	2.65611300	-0.06936000	-3.59447600
O	-0.10951897	-3.53895393	-0.95303846	H	2.54345700	1.53753900	4.29972000
				H	2.65611300	-0.06936000	3.59447600
				H	2.47233800	1.34661300	2.54944800
2Cr-trans-Cs				2Cr-C1			
O	2.11786300	2.09358700	0.00000000	O	-0.08441800	-3.01883000	-0.83829000
N	1.29843100	1.23236000	0.00000000	Cr	-0.00149700	-0.06883000	-0.28087700
Cr	0.02501200	0.14829600	0.00000000	P	2.27220100	0.15566500	0.16357000
H	-1.35911800	-0.79933700	0.00000000	P	-2.28181500	0.16459500	0.08878000
P	-0.08062500	-0.31795000	2.27326700	C	2.44096800	-0.33129500	1.96851200
P	-0.08062500	-0.31795000	-2.27326700	C	-2.41823300	-0.02012200	1.94491000
C	0.95814600	-1.87456800	2.43420700	H	2.56400800	0.57684000	2.56351600
C	0.95814600	-1.87456800	-2.43420700	H	-2.33165300	0.98212900	2.37635000
H	0.27235800	-2.72814900	2.44651100	H	3.33019400	-0.94180900	2.13658900
H	0.27235800	-2.72814900	-2.44651100	H	-3.38322900	-0.42273400	2.25880500
H	1.52636300	-1.90778700	3.36568900	C	1.18823100	-1.07624800	2.41018800
H	1.52636300	-1.90778700	-3.36568900	C	-1.27372300	-0.88856700	2.44545600
C	1.88038700	-1.97639100	1.23038200	H	1.16691400	-1.17418600	3.50545800
C	1.88038700	-1.97639100	-1.23038200	H	-1.26392800	-0.91611000	3.54496100
H	2.38468500	-2.95372600	1.21242100	H	1.16852700	-2.08250000	1.98568500
H	2.38468500	-2.95372600	-1.21242100	H	-1.38227800	-1.91555300	2.08940100
H	2.65152200	-1.20363700	1.26670100	N	-0.00392100	-0.36827300	1.92488900
H	2.65152200	-1.20363700	-1.26670100	C	-3.21356800	1.76832400	-0.27598300
N	1.10495400	-1.76395700	0.00000000	C	3.06115800	1.86555200	0.09289300
H	0.32399700	-2.41534000	0.00000000	H	-3.50644200	1.64054000	-1.32433200
C	-1.68731000	-0.92090600	-3.05200000	H	4.09499000	1.74649300	0.43127300
C	-1.68731000	-0.92090600	3.05200000	C	-3.53414500	-1.06129400	-0.61122000
H	-1.88044600	-1.81079500	-2.44106700	C	3.57952500	-0.89874100	-0.70887800
H	-1.88044600	-1.81079500	2.44106700	C	-3.49324800	-2.43101900	0.05947200
C	0.68208900	0.84773000	-3.53728900	C	5.03079500	-0.52107400	-0.41743900
C	0.68208900	0.84773000	3.53728900	O	0.05827500	0.61955800	-3.03265800
C	2.19769200	0.95055400	-3.37436900	H	3.37529000	-0.71868200	-1.76986500
C	2.19769200	0.95055400	3.37436900	H	-4.52342100	-0.62579800	-0.43457000
C	-1.24748300	1.45223800	0.00000000	C	3.35973500	-2.38612600	-0.44239100
O	-2.06468900	2.27281100	0.00000000	C	-3.32325100	-1.18838900	-2.11960500

H 0.46895500	0.42270900	4.52400200	H 2.34626100	-2.70556100	-0.67355600
H 0.46895500	0.42270900	-4.52400200	H -3.37240200	-0.22521200	-2.63277700
C 0.04545800	2.23340100	3.44111300	H 3.57230100	-2.64294400	0.59994400
C 0.04545800	2.23340100	-3.44111300	H -2.34964000	-1.62920800	-2.34018200
H -1.03160100	2.21470900	3.61165200	H 4.04390400	-2.97498100	-1.06039400
H -1.03160100	2.21470900	-3.61165200	H -4.09379000	-1.83264200	-2.55383300
H 0.21939600	2.67093500	2.45626700	C -4.48404200	1.95071600	0.55558100
H 0.21939600	2.67093500	-2.45626700	C 2.38015600	2.88742400	0.99620300
H 0.48788800	2.89877500	4.18881200	H -4.24726400	2.15512400	1.60305700
H 0.48788800	2.89877500	-4.18881200	H 1.32642500	2.99246700	0.73122300
C -2.86265100	0.02714000	-2.83759500	H -5.14852600	1.08496200	0.52482900
C -2.86265100	0.02714000	2.83759500	H 2.44175000	2.62404300	2.05525600
H -2.76334300	0.94256600	-3.42466800	H -5.05180400	2.80834000	0.18245400
H -2.76334300	0.94256600	3.42466800	H 2.86798400	3.86015300	0.87955400
H -2.96408500	0.30271900	-1.78871500	C -2.33134900	3.00738800	-0.18915800
H -2.96408500	0.30271900	1.78871500	C 3.05708000	2.35255200	-1.35596200
H -3.79077700	-0.45968800	-3.15297800	H -1.44840900	2.91556500	-0.81923000
H -3.79077700	-0.45968800	3.15297800	H 3.58830800	1.67636200	-2.02936500
C -1.57016300	-1.34616900	-4.51341700	H -1.98191800	3.17963700	0.83293600
C -1.57016300	-1.34616900	4.51341700	H 2.03359600	2.45150300	-1.72381900
H -0.73537600	-2.02875000	-4.69014200	H -2.90182200	3.88963600	-0.49752100
H -0.73537600	-2.02875000	4.69014200	H 3.53817400	3.33272300	-1.42583500
H -1.44613800	-0.48440300	-5.17392400	H -0.02455800	1.48366200	0.23512500
H -1.44613800	-0.48440300	5.17392400	H 0.06955100	0.60982900	2.19039400
H -2.48485400	-1.85926100	-4.82614700	H -4.24537800	-3.08364700	-0.39454900
H -2.48485400	-1.85926100	4.82614700	H -2.52420800	-2.91422200	-0.07118700
H 2.59812700	1.63347100	-4.12995200	H -3.71576800	-2.38068400	1.12785100
H 2.46816200	1.34950600	-2.39571100	H 5.70068600	-1.21985800	-0.92792700
H 2.70197700	-0.00861800	-3.51030300	H 5.28737500	0.48138600	-0.76114700
H 2.59812700	1.63347100	4.12995200	H 5.25922000	-0.58134400	0.65130900
H 2.70197700	-0.00861800	3.51030300	N 0.03062600	0.32215100	-1.89279000
H 2.46816200	1.34950600	2.39571100	C -0.03886600	-1.88552600	-0.58044600
1Mo-cis-Cs			1Mo-trans-Cs		
C 0.31479600	1.95278100	0.00000000	C -2.04409300	-0.65031000	0.00000000
C -1.08979000	0.99116200	-3.45380000	C 1.12664700	1.06144200	3.37489100
C -1.08979000	0.99116200	3.45380000	C 1.12664700	1.06144200	-3.37489100
H -1.29556000	0.51489900	-4.41904700	H 1.31577500	0.64922300	4.37233900
H -1.29556000	0.51489900	4.41904700	H 1.31577500	0.64922300	-4.37233900
C -2.42224400	1.30984100	-2.77767400	C 2.46960000	1.31528500	2.69274100
C -2.42224400	1.30984100	2.77767400	C 2.46960000	1.31528500	-2.69274100
H -2.26780800	1.71170200	-1.77321900	H 2.33009600	1.64543400	1.65996200
H -2.26780800	1.71170200	1.77321900	H 2.33009600	1.64543400	-1.65996200
H -3.06800200	0.43426500	-2.69693300	H 3.10599200	0.42934900	2.68248300
H -3.06800200	0.43426500	2.69693300	H 3.10599200	0.42934900	-2.68248300
H -2.96060400	2.06436600	-3.35881400	H 3.01051700	2.10397400	3.22405500
H -2.96060400	2.06436600	3.35881400	H 3.01051700	2.10397400	-3.22405500
C -0.28868000	2.26893800	-3.69004000	C 0.34248900	2.36509400	3.51173800
C -0.28868000	2.26893800	3.69004000	C 0.34248900	2.36509400	-3.51173800
H -0.91007900	2.99972800	-4.21645900	H 0.96130100	3.11523900	4.01352000
H -0.91007900	2.99972800	4.21645900	H 0.96130100	3.11523900	-4.01352000
H 0.59905900	2.09744500	-4.29869500	H -0.56683800	2.24585200	4.10081600
H 0.59905900	2.09744500	4.29869500	H -0.56683800	2.24585200	-4.10081600
H 0.02897800	2.72109400	-2.74857800	H 0.05977800	2.76497300	2.53573200
H 0.02897800	2.72109400	2.74857800	H 0.05977800	2.76497300	-2.53573200
C 1.29005400	-0.85955800	-3.51502000	C -1.24787900	-0.78019400	3.56899400
C 1.29005400	-0.85955800	3.51502000	C -1.24787900	-0.78019400	-3.56899400
H 1.57839200	-1.77569900	-2.98565700	H -1.54478000	-1.71922300	3.08645300
H 1.57839200	-1.77569900	2.98565700	H -1.54478000	-1.71922300	-3.08645300
C 2.49893600	0.07361200	-3.49304500	C -2.45622500	0.15238000	3.52010300
C 2.49893600	0.07361200	3.49304500	C -2.45622500	0.15238000	-3.52010300
H 3.36434600	-0.44123800	-3.92060700	H -3.32748000	-0.34966000	3.95045000
H 3.36434600	-0.44123800	3.92060700	H -3.32748000	-0.34966000	-3.95045000

H 2.76030100	0.38026300	-2.48127700	H -2.70415600	0.43925500	2.49777900
H 2.76030100	0.38026300	2.48127700	H -2.70415600	0.43925500	-2.49777900
H 2.33103700	0.97162600	-4.08979700	H -2.29025600	1.06363900	4.09741800
H 2.33103700	0.97162600	4.08979700	H -2.29025600	1.06363900	-4.09741800
C 0.88844600	-1.23031500	-4.94049500	C -0.82391300	-1.08546400	5.00306900
C 0.88844600	-1.23031500	4.94049500	C -0.82391300	-1.08546400	-5.00306900
H 0.60530300	-0.34759500	-5.51939600	H -0.53570800	-0.17683800	5.53770700
H 0.60530300	-0.34759500	5.51939600	H -0.53570800	-0.17683800	-5.53770700
H 0.05626000	-1.93708800	-4.97125300	H 0.01189600	-1.78714500	5.05198200
H 0.05626000	-1.93708800	4.97125300	H 0.01189600	-1.78714500	-5.05198200
H 1.73401100	-1.69587000	-5.45586800	H -1.65875300	-1.53087200	5.55265800
H 1.73401100	-1.69587000	5.45586800	H -1.65875300	-1.53087200	-5.55265800
C -1.24886300	-1.76787900	-2.45725100	C 1.25077400	-1.74452300	2.45786300
C -1.24886300	-1.76787900	2.45725100	C 1.25077400	-1.74452300	-2.45786300
H -1.88403100	-1.80951000	-3.34663000	H 1.88327000	-1.78351600	3.34920500
H -1.88403100	-1.80951000	3.34663000	H 1.88327000	-1.78351600	-3.34920500
H -0.57427300	-2.62846500	-2.48900000	H 0.56855100	-2.59852300	2.49863300
H -0.57427300	-2.62846500	2.48900000	H 0.56855100	-2.59852300	-2.49863300
C -2.07799500	-1.83349500	-1.18191100	C 2.08454400	-1.83117600	1.18428900
C -2.07799500	-1.83349500	1.18191100	C 2.08454400	-1.83117600	-1.18428900
H -3.01360300	-1.26593000	-1.31067100	H 3.03340700	-1.28794200	1.31850900
H -3.01360300	-1.26593000	1.31067100	H 3.03340700	-1.28794200	-1.31850900
H -2.39263000	-2.87898700	-1.03624600	H 2.37401700	-2.88493600	1.04185300
H -2.39263000	-2.87898700	1.03624600	H 2.37401700	-2.88493600	-1.04185300
N 2.03306700	-0.12179200	0.00000000	N -0.77162200	1.73415000	0.00000000
N -1.35613400	-1.36984600	0.00000000	N 1.38317400	-1.34921600	0.00000000
O 3.19218400	-0.36923300	0.00000000	O -1.02303700	2.89147200	0.00000000
O 0.33360700	3.11290000	0.00000000	O -3.11393300	-1.09953000	0.00000000
P -0.14110400	-0.27808100	-2.44438100	P 0.15546200	-0.24571400	2.43891400
P -0.14110400	-0.27808100	2.44438100	P 0.15546200	-0.24571400	-2.43891400
Mo 0.22426000	-0.01285300	0.00000000	Mo -0.20452700	0.00315500	0.00000000
1Mo-C1			1Mo-C1-triplet		
C -2.47778200	-0.61287200	1.97457900	C -2.49962612	-0.55618026	1.94831754
H -2.56314200	0.30780000	2.55694900	H -2.66107345	0.38097335	2.48592840
H -3.34828500	-1.23341800	2.20458200	H -3.33059475	-1.22597297	2.18561314
C -1.17790200	-1.31744400	2.34668900	C -1.16811641	-1.15617535	2.37915340
H -1.06129400	-1.25963900	3.44039600	H -1.09046097	-1.07109384	3.47410635
H -1.25892700	-2.39278800	2.11900400	H -1.15917638	-2.23849895	2.16945053
C 1.18634600	-1.19538600	2.41221800	C 1.17470527	-0.94254510	2.50812686
H 1.36223800	-2.26812600	2.23079700	H 1.29878470	-2.03472786	2.42499526
H 1.02039400	-1.10671500	3.49757900	H 1.01775749	-0.74690121	3.58036747
C 2.44059600	-0.40262600	2.06061100	C 2.45602281	-0.24612211	2.07158746
H 3.34667400	-0.93898600	2.35530600	H 3.34088650	-0.79033856	2.41223062
H 2.42921900	0.54564100	2.60241300	H 2.49121705	0.75407910	2.50796545
C -3.52076000	1.44441700	0.12477100	C -3.65785531	1.30783776	-0.03112442
H -3.50216900	1.71809900	-0.93535200	H -3.57330419	1.57847978	-1.08884697
C -4.96795500	1.21643400	0.55444200	C -5.10755679	0.93626545	0.27358101
H -5.02937800	0.88460300	1.59467500	H -5.22315129	0.58965750	1.30439040
H -5.48118700	0.48017800	-0.06627200	H -5.49556653	0.16213947	-0.38993910
H -5.52931700	2.15272200	0.47950800	H -5.74663902	1.81650276	0.15490129
C -2.88743800	2.59345100	0.90690700	C -3.22284695	2.51724745	0.79336651
H -3.45158100	3.51382800	0.73135100	H -3.81412743	3.39089665	0.50544334
H -1.85511700	2.77074900	0.60539400	H -2.17039192	2.75747959	0.64439673
H -2.90130000	2.40594300	1.98393200	H -3.38828029	2.35394937	1.86166584
C -3.45409900	-1.38669400	-0.70432000	C -3.30146088	-1.53549359	-0.72346752
H -4.42493500	-1.42389400	-0.19826200	H -4.28016796	-1.63806559	-0.24248753
C -3.66491600	-0.99553200	-2.16478800	C -3.50113159	-1.22402698	-2.20490550
H -2.71070100	-0.88639500	-2.68460600	H -2.54406290	-1.07147421	-2.70763368
H -4.21518600	-0.05813900	-2.26983700	H -4.11263184	-0.33373150	-2.36599400
H -4.23806200	-1.77200300	-2.67991000	H -4.00512172	-2.06158984	-2.69618941
C -2.79867400	-2.76052000	-0.58801500	C -2.53512114	-2.84199169	-0.53507246
H -3.39623600	-3.50410900	-1.12365200	H -3.04828796	-3.65245400	-1.06128154

H -2.71446800	-3.09122600	0.44911200	H -2.45909363	-3.12850318	0.51567108
H -1.79849600	-2.75851000	-1.02629100	H -1.52429281	-2.76654387	-0.94212269
C 3.47488500	1.58220400	0.12270300	C 3.61828667	1.39028050	-0.11553351
H 4.43643400	1.35424900	0.59587200	H 4.59812711	1.04310726	0.22834769
C 3.70567600	1.93198000	-1.34718500	C 3.67643103	1.64536943	-1.62156342
H 2.75755800	2.11650700	-1.85680900	H 2.70217159	1.96265823	-1.99957863
H 4.23313700	1.14435500	-1.88873000	H 3.98337288	0.76146195	-2.18474210
H 4.30732900	2.84232900	-1.42265300	H 4.39671171	2.43975161	-1.83728974
C 2.83317100	2.75581400	0.85937000	C 3.26960560	2.66831125	0.64197599
H 3.48096300	3.63408500	0.78210000	H 3.96773806	3.46056339	0.35613571
H 2.68161100	2.55604100	1.92178300	H 3.34435058	2.54685854	1.72407271
H 1.86794500	3.01469100	0.42085500	H 2.26178274	3.01129076	0.40539009
C 3.46509300	-1.28791000	-0.58284900	C 3.25466377	-1.50670613	-0.51219529
H 3.36902300	-1.04525800	-1.64639300	H 3.11710816	-1.35722549	-1.58822450
C 2.84864600	-2.66844800	-0.36194500	C 2.51802122	-2.78891258	-0.12711808
H 3.32706200	-3.40145800	-1.01747100	H 2.86982061	-3.62059683	-0.74390118
H 1.77841200	-2.67566200	-0.57538200	H 1.43954640	-2.69622763	-0.27044092
H 2.99364800	-3.00681100	0.66717400	H 2.70347484	-3.05488717	0.91664692
C 4.94357000	-1.28323900	-0.20417400	C 4.74723741	-1.62695557	-0.21724097
H 5.08656000	-1.46533800	0.86470000	H 4.94446573	-1.68722607	0.85699348
H 5.44061400	-0.34510500	-0.45558400	H 5.32532079	-0.79454237	-0.62119245
H 5.46557300	-2.08246300	-0.73925100	H 5.13967491	-2.54334527	-0.66851544
N -0.05314600	1.73711000	-1.08604500	N -0.00062592	2.14288034	-0.47922483
N -0.00333100	-0.74274500	1.69523200	N -0.00825757	-0.50970969	1.76659417
O -0.09611000	2.82623700	-1.54963500	O -0.00459121	3.10809838	-1.18071403
P -2.44085900	-0.09123200	0.19514300	P -2.43949926	-0.11595050	0.14733914
P 2.42818200	0.03376800	0.25917700	P 2.41198325	-0.00149437	0.23605573
Mo -0.00328600	0.15370300	-0.18949900	C 0.15386339	-0.59267067	-1.91912552
C 0.09213700	-0.78191300	-1.90474700	O 0.27728927	-1.12902382	-2.94881418
O 0.16802900	-1.36001500	-2.90821300	Mo -0.00650663	0.26942353	-0.15917114
2Mo-cis-Cs			2Mo-trans-Cs		
C -1.59528800	1.30640100	0.00000000	C -1.50328500	-1.56474200	0.00000000
C -0.70713100	0.73039400	-3.72854600	C 0.72985500	-0.78056500	-3.66708100
C -0.70713100	0.73039400	3.72854600	C 0.72985500	-0.78056500	3.66708100
H -0.52511600	0.22740700	-4.68430800	H 0.62551300	-0.28489400	-4.63835300
H -0.52511600	0.22740700	4.68430800	H 0.62551300	-0.28489400	4.63835300
C -2.21478600	0.86140000	-3.53014000	C 2.21622700	-0.98861900	-3.38475200
C -2.21478600	0.86140000	3.53014000	C 2.21622700	-0.98861900	3.38475200
H -2.45094500	1.33289300	-2.57516400	H 2.37555200	-1.44450700	-2.40631800
H -2.45094500	1.33289300	2.57516400	H 2.37555200	-1.44450700	2.40631800
H -2.73141300	-0.09994700	-3.57631800	H 2.78685000	-0.05847100	-3.43147300
H -2.73141300	-0.09994700	3.57631800	H 2.78685000	-0.05847100	3.43147300
H -2.63374900	1.49009800	-4.32166300	H 2.63846900	-1.66273100	-4.13613000
H -2.63374900	1.49009800	4.32166300	H 2.63846900	-1.66273100	4.13613000
C -0.05047200	2.10938800	-3.75126000	C 0.00163300	-2.12252100	-3.70537200
C -0.05047200	2.10938800	3.75126000	C 0.00163300	-2.12252100	3.70537200
H -0.53708200	2.74367500	-4.49828000	H 0.48321600	-2.78653000	-4.42952500
H -0.53708200	2.74367500	4.49828000	H 0.48321600	-2.78653000	4.42952500
H 1.01080100	2.06357400	-3.99848900	H -1.04530700	-2.02280300	-3.99439700
H 1.01080100	2.06357400	3.99848900	H -1.04530700	-2.02280300	3.99439700
H -0.14505600	2.59841700	-2.77878000	H 0.03406600	-2.60732900	-2.72736600
H -0.14505600	2.59841700	2.77878000	H 0.03406600	-2.60732900	2.72736600
C 1.69716700	-0.95607100	-3.14906900	C -1.61069400	1.04855000	-3.20536000
C 1.69716700	-0.95607100	3.14906900	C -1.61069400	1.04855000	3.20536000
H 1.88545900	-1.82939300	-2.51395200	H -1.78017700	1.93715000	-2.58609900
H 1.88545900	-1.82939300	2.51395200	H -1.78017700	1.93715000	2.58609900
C 2.85285200	0.01261000	-2.91619900	C -2.82599100	0.14524800	-3.02286200
C 2.85285200	0.01261000	2.91619900	C -2.82599100	0.14524800	3.02286200
H 3.79945700	-0.47208100	-3.17421800	H -3.72951500	0.67467500	-3.34058800
H 3.79945700	-0.47208100	3.17421800	H -3.72951500	0.67467500	3.34058800
H 2.89928900	0.31764200	-1.87022300	H -2.94740700	-0.14051800	-1.97823300
H 2.89928900	0.31764200	1.87022300	H -2.94740700	-0.14051800	1.97823300

H 2.76928300	0.90929300	-3.53386000	H -2.75606000	-0.76480600	-3.62221000
H 2.76928300	0.90929300	3.53386000	H -2.75606000	-0.76480600	3.62221000
C 1.61069400	-1.40675200	-4.60395700	C -1.43622000	1.48328200	-4.65772000
C 1.61069400	-1.40675200	4.60395700	C -1.43622000	1.48328200	4.65772000
H 1.48388800	-0.55886800	-5.28173600	H -1.31963600	0.62412800	-5.32299600
H 1.48388800	-0.55886800	5.28173600	H -1.31963600	0.62412800	5.32299600
H 0.78917500	-2.10586700	-4.78120600	H -0.57500000	2.14055200	-4.80168900
H 0.78917500	-2.10586700	4.78120600	H -0.57500000	2.14055200	4.80168900
H 2.53775400	-1.91124500	-4.89335200	H -2.32384900	2.02895800	-4.99216800
H 2.53775400	-1.91124500	4.89335200	H -2.32384900	2.02895800	4.99216800
C -0.94162500	-1.91746000	-2.44204400	C 1.04839100	1.88497900	-2.45005200
C -0.94162500	-1.91746000	2.44204400	C 1.04839100	1.88497900	2.45005200
H -1.51339800	-2.00064900	-3.36864400	H 1.63619300	1.93079900	-3.36953100
H -1.51339800	-2.00064900	3.36864400	H 1.63619300	1.93079900	3.36953100
H -0.23787800	-2.75577200	-2.42569700	H 0.39045300	2.76026000	-2.44932500
H -0.23787800	-2.75577200	2.42569700	H 0.39045300	2.76026000	2.44932500
C -1.86965900	-2.00926900	-1.23791700	C 1.96396300	1.93556700	-1.23472300
C -1.86965900	-2.00926900	1.23791700	C 1.96396300	1.93556700	1.23472300
H -2.64986200	-1.24650400	-1.28981400	H 2.70623100	1.13527700	-1.27448000
H -2.64986200	-1.24650400	1.28981400	H 2.70623100	1.13527700	1.27448000
H -2.36441700	-2.99133200	-1.21810700	H 2.50564900	2.89270600	-1.21098000
H -2.36441700	-2.99133200	1.21810700	H 2.50564900	2.89270600	1.21098000
N 1.15489700	1.68900600	0.00000000	N 1.23819000	-1.49715300	0.00000000
N -1.10894100	-1.78736900	0.00000000	N 1.18464100	1.75061800	0.00000000
H -0.30445600	-2.41009800	0.00000000	H 0.42116800	2.42349600	0.00000000
O 1.86142800	2.63463900	0.00000000	O 2.01439500	-2.39521000	0.00000000
O -2.56349300	1.94841900	0.00000000	O -2.36077900	-2.34299300	0.00000000
P 0.08223400	-0.34208200	-2.39920400	P -0.05620600	0.36005700	-2.39656300
P 0.08223400	-0.34208200	2.39920400	P -0.05620600	0.36005700	2.39656300
Mo 0.09500100	0.22303700	0.00000000	Mo -0.06922200	-0.20668300	0.00000000
H 1.41709500	-1.02289800	0.00000000	H -1.45313700	1.00043200	0.00000000
2Mo-C1			1W-cis-Cs		
C 0.01615800	-1.97281500	-0.73260900	C -0.25417300	-1.95304300	0.00000000
C 3.70262500	-1.02130600	-0.48552400	C 1.11779800	-0.98184700	-3.44307900
C -3.66117200	-1.10634000	-0.48358700	C 1.11779800	-0.98184700	3.44307900
H 3.53635100	-0.99669000	-1.56759500	H 1.30460100	-0.50862800	-4.41369100
H -4.63095500	-0.82117100	-0.06493000	H 1.30460100	-0.50862800	4.41369100
C 5.15861900	-0.65773600	-0.20142500	C 2.46250100	-1.27460200	-2.77968900
C -3.36270200	-2.53380000	-0.03830300	C 2.46250100	-1.27460200	2.77968900
H 5.35237300	-0.56309600	0.87168600	H 2.32483700	-1.67444000	-1.77197500
H -2.40215300	-2.88300800	-0.41531300	H 2.32483700	-1.67444000	1.77197500
H 5.46743900	0.27024200	-0.68340700	H 3.09512500	-0.38835800	-2.71055500
H -3.36579600	-2.64031200	1.04922200	H 3.09512500	-0.38835800	2.71055500
H 5.81310000	-1.45079800	-0.57596600	H 3.00695400	-2.02314000	-3.36278500
H -4.13484500	-3.20443600	-0.42787500	H 3.00695400	-2.02314000	3.36278500
C 3.41164700	-2.44076900	-0.00406100	C 0.33339400	-2.27325600	-3.66003400
C -3.72244700	-1.00594700	-2.00617600	C 0.33339400	-2.27325600	3.66003400
H 4.06274100	-3.14776200	-0.52613300	H 0.96014500	-2.99792600	-4.18854200
H -4.44730500	-1.72261000	-2.40350400	H 0.96014500	-2.99792600	4.18854200
H 2.38280600	-2.74023800	-0.19348600	H -0.56365500	-2.11970600	-4.25968700
H -4.02119700	-0.01183600	-2.34683500	H -0.56365500	-2.11970600	4.25968700
H 3.61638100	-2.54966800	1.06532000	H 0.03385600	-2.72260500	-2.71151800
H -2.74831900	-1.23005700	-2.44739700	H 0.03385600	-2.72260500	2.71151800
C 3.28444700	1.85046600	-0.07063600	C -1.29263800	0.83541300	-3.48256000
C -3.34629100	1.77173200	-0.06218800	C -1.29263800	0.83541300	3.48256000
H 4.30125700	1.72446000	0.31308100	H -1.59079600	1.74593000	-2.94911400
H -3.24476200	1.94209200	-1.13964200	H -1.59079600	1.74593000	2.94911400
C 2.62941400	3.00535000	0.67775300	C -2.48411700	-0.11931500	-3.44757800
C -4.83229500	1.73575400	0.29213800	C -2.48411700	-0.11931500	3.44757800
H 3.15340600	3.93563200	0.43755800	H -3.36185900	0.38159100	-3.86640000
H -5.26190700	2.73410000	0.16524800	H -3.36185900	0.38159100	3.86640000
H 2.67366300	2.88348400	1.76287000	H -2.73063600	-0.42927700	-2.43330400

H -5.40648000	1.05736000	-0.33983200	H -2.73063600	-0.42927700	2.43330400
H 1.58171100	3.10734500	0.38980700	H -2.30652100	-1.01368600	-4.04687900
H -4.99310200	1.44756400	1.33542700	H -2.30652100	-1.01368600	4.04687900
C 3.34320900	2.14903300	-1.56912900	C -0.91157800	1.21244200	-4.91205100
C -2.65555500	2.93213400	0.64858700	C -0.91157800	1.21244200	4.91205100
H 2.33635600	2.25588800	-1.97878500	H -0.62021500	0.33436100	-5.49389100
H -2.82049600	2.89476600	1.73022700	H -0.62021500	0.33436100	5.49389100
H 3.85173000	1.36570400	-2.13582300	H -0.09181400	1.93322200	-4.95213400
H -1.58095900	2.92660100	0.46126900	H -0.09181400	1.93322200	4.95213400
H 3.88167900	3.08498000	-1.74452300	H -1.77051500	1.66347500	-5.41791900
H -3.07132700	3.88017200	0.29534200	H -1.77051500	1.66347500	5.41791900
C 2.45487600	-0.07645600	2.02635400	C 1.25104200	1.78434000	-2.46083800
C -2.45039300	-0.13955400	2.02753400	C 1.25104200	1.78434000	2.46083800
H 3.37921500	-0.57083100	2.33358500	H 1.88853300	1.82852900	-3.34800000
H -3.36164100	-0.65751100	2.33501900	H 1.88853300	1.82852900	3.34800000
H 2.44439900	0.90424200	2.50837900	H 0.56651100	2.63668800	-2.49825700
H -2.46304200	0.84261800	2.50843300	H 0.56651100	2.63668800	2.49825700
C 1.24824700	-0.88486300	2.48877900	C 2.07571600	1.86304900	-1.18339600
C -1.22249700	-0.91633100	2.48885900	C 2.07571600	1.86304900	1.18339600
H 1.30231000	-1.90919200	2.11365400	H 3.02227900	1.31555000	-1.30958000
H -1.24973900	-1.94125800	2.11204100	H 3.02227900	1.31555000	1.30958000
H 1.22858900	-0.93349200	3.58740400	H 2.36492100	2.91318200	-1.02861800
H -1.20108000	-0.96560800	3.58739800	H 2.36492100	2.91318200	1.02861800
N -0.01258800	0.42991800	-2.10602300	N -1.99143200	0.11342100	0.00000000
N 0.00499100	-0.28965900	1.97569800	N 1.36335200	1.37567400	0.00000000
H -0.00695100	0.69692400	2.22346400	O -3.15717400	0.36153700	0.00000000
O -0.02546300	0.73998700	-3.24439500	O -0.24525100	-3.11781500	0.00000000
O 0.03809200	-3.10265600	-1.00395300	P 0.16257600	0.28099700	-2.43282300
P 2.41256500	0.19966900	0.17049500	P 0.16257600	0.28099700	2.43282300
P -2.41511800	0.14071800	0.17305800	W -0.18142200	0.00825300	0.00000000
Mo 0.00102700	-0.00056000	-0.34948000			
H 0.01852800	1.69136100	0.25035000			
1W-trans-Cs			1W-C1		
C -2.05449700	0.54924500	0.00000000	C -2.48095400	-0.62324400	2.00091500
C 1.15184800	-1.05023400	-3.35568600	H -2.57923600	0.30022500	2.57645800
C 1.15184800	-1.05023400	3.35568600	H -3.34579400	-1.25162800	2.22930300
H 1.33494300	-0.64224700	-4.35606700	C -1.17639000	-1.31333400	2.38378600
H 1.33494300	-0.64224700	4.35606700	H -1.05145900	-1.22838700	3.47350500
C 2.49776600	-1.28537700	-2.67291400	H -1.25085700	-2.39273300	2.17979400
C 2.49776600	-1.28537700	2.67291400	C 1.19010300	-1.18773100	2.44695600
H 2.36083100	-1.61346300	-1.63922100	H 1.36083100	-2.26390900	2.28927800
H 2.36083100	-1.61346300	1.63922100	H 1.01527100	-1.07276300	3.52715500
H 3.12464000	-0.39246600	-2.66660800	C 2.44877000	-0.40719700	2.08360000
H 3.12464000	-0.39246600	2.66660800	H 3.35125700	-0.95071100	2.37501600
H 3.04731600	-2.07003300	-3.20120800	H 2.44978500	0.54439700	2.61946100
H 3.04731600	-2.07003300	3.20120800	C -3.49798400	1.42563400	0.11883500
C 0.38034600	-2.36262900	-3.48216600	H -3.44515500	1.69948600	-0.93998900
C 0.38034600	-2.36262900	3.48216600	C -4.95785300	1.19946700	0.50455500
H 1.00601900	-3.10764900	-3.98310000	H -5.05130500	0.86544800	1.54179500
H 1.00601900	-3.10764900	3.98310000	H -5.45468900	0.46662700	-0.13315600
H -0.53177000	-2.25573900	-4.06912200	H -5.51347200	2.13780900	0.41549300
H -0.53177000	-2.25573900	4.06912200	C -2.88657200	2.57229800	0.92139300
H 0.10577700	-2.76127600	-2.50358600	H -3.44361700	3.49324300	0.72747100
H 0.10577700	-2.76127600	2.50358600	H -1.84566400	2.74901600	0.65177800
C -1.24524900	0.76625300	-3.55308100	H -2.93648000	2.38495000	1.99742000
C -1.24524900	0.76625300	3.55308100	C -3.42926400	-1.41685800	-0.68370000
H -1.55718900	1.69823000	-3.06635800	H -4.40473100	-1.45319600	-0.18654000
H -1.55718900	1.69823000	3.06635800	C -3.62494600	-1.03423700	-2.14843200
C -2.43660200	-0.18773600	-3.50518200	H -2.66524000	-0.92643900	-2.65791400
C -2.43660200	-0.18773600	3.50518200	H -4.17568500	-0.09845300	-2.26460100
H -3.31958200	0.30542300	-3.92149100	H -4.19137600	-1.81490400	-2.66459800
H -3.31958200	0.30542300	3.92149100	C -2.76945700	-2.78714100	-0.55241700

H -2.67097300	-0.49118700	-2.48462900	H -3.35958600	-3.53672700	-1.08783000
H -2.67097300	-0.49118700	2.48462900	H -2.69248000	-3.11096100	0.48758500
H -2.25985300	-1.08796600	-4.09634400	H -1.76601100	-2.78313500	-0.98330800
H -2.25985300	-1.08796600	4.09634400	C 3.45315200	1.56915800	0.11378100
C -0.82768400	1.08215200	-4.98674500	H 4.42460600	1.34437700	0.56787600
C -0.82768400	1.08215200	4.98674500	C 3.65240200	1.91084100	-1.36272200
H -0.52308000	0.17997600	-5.52318200	H 2.69351000	2.09193900	-1.85253000
H -0.52308000	0.17997600	5.52318200	H 4.16969900	1.12088000	-1.91070100
H -0.00547500	1.79975700	-5.03566800	H 4.25162200	2.82125400	-1.45445800
H -0.00547500	1.79975700	5.03566800	C 2.82463100	2.74502700	0.85806700
H -1.67149700	1.51246700	-5.53451400	H 3.47532300	3.62019400	0.77063800
H -1.67149700	1.51246700	5.53451400	H 2.68793500	2.54731000	1.92294300
C 1.25023300	1.76604600	-2.46351400	H 1.85527200	3.00760800	0.43178300
C 1.25023300	1.76604600	2.46351400	C 3.44446300	-1.30910800	-0.56674600
H 1.88940800	1.80103600	-3.34978200	H 3.33038000	-1.07360400	-1.63000700
H 1.88940800	1.80103600	3.34978200	C 2.83237400	-2.68819800	-0.32671200
H 0.56125300	2.61374400	-2.51764100	H 3.30460300	-3.42633100	-0.98088500
H 0.56125300	2.61374400	2.51764100	H 1.76011900	-2.69780100	-0.53046300
C 2.07325600	1.86883300	-1.18482600	H 2.98836900	-3.01796400	0.70373000
C 2.07325600	1.86883300	1.18482600	C 4.92817600	-1.29802900	-0.21007200
H 3.02987700	1.33893500	-1.30785400	H 5.08795800	-1.47057500	0.85808500
H 3.02987700	1.33893500	1.30785400	H 5.41910400	-0.36108700	-0.47738800
H 2.34277600	2.92583800	-1.03782000	H 5.44375900	-2.10065400	-0.74617100
H 2.34277600	2.92583800	1.03782000	N -0.05602100	1.73166000	-1.00381300
N -0.62552600	-1.75250500	0.00000000	N -0.00078400	-0.75300100	1.71217100
N 1.37260300	1.37498300	0.00000000	O -0.09964900	2.84657600	-1.42161900
O -0.78458400	-2.93318900	0.00000000	P -2.42887600	-0.11411700	0.21870300
O -3.14969700	0.94530300	0.00000000	P 2.41873600	0.01707000	0.28005600
P 0.17160300	0.25586800	-2.42980900	W -0.00250300	0.12123400	-0.15953900
P 0.17160300	0.25586800	2.42980900	C 0.09460500	-0.77393800	-1.89416900
W -0.17878700	0.01215900	0.00000000	O 0.17050400	-1.35026400	-2.90357700
1W-C1-triplet			2W-cis-Cs		
C -2.50060210	-0.52513064	1.98115071	C 1.56680100	1.25913600	0.00000000
H -2.66959460	0.42898299	2.48536515	C 0.69233400	0.76524500	3.69066600
H -3.32720996	-1.19281579	2.23725617	C 0.69233400	0.76524500	-3.69066600
C -1.16563012	-1.10209737	2.43115324	H 0.49268000	0.30140300	4.66250400
H -1.07846982	-0.96586164	3.51897841	H 0.49268000	0.30140300	-4.66250400
H -1.15405113	-2.19162554	2.26836510	C 2.20285200	0.90321500	3.51933900
C 1.17569177	-0.88104902	2.55168793	C 2.20285200	0.90321500	-3.51933900
H 1.29183721	-1.97621159	2.52336022	H 2.45533400	1.33454700	2.54971900
H 1.01074020	-0.62927819	3.60976179	H 2.45533400	1.33454700	-2.54971900
C 2.46439689	-0.21659213	2.08821058	H 2.72866000	-0.04872300	3.62213400
H 3.34272685	-0.76443601	2.43880159	H 2.72866000	-0.04872300	-3.62213400
H 2.51789257	0.79613516	2.49233618	H 2.59629700	1.57217000	4.29063500
C -3.63648334	1.26847907	-0.08449564	H 2.59629700	1.57217000	-4.29063500
H -3.51708769	1.51189049	-1.14537601	C 0.02357500	2.13796000	3.63892600
C -5.09415013	0.89855358	0.18241242	C 0.02357500	2.13796000	-3.63892600
H -5.24220852	0.57638981	1.21704805	H 0.47880500	2.80243500	4.37940000
H -5.45955179	0.10843801	-0.47481980	H 0.47880500	2.80243500	-4.37940000
H -5.73013710	1.77437632	0.02267757	H -1.04571400	2.09263500	3.84821700
C -3.23349746	2.49949966	0.72384422	H -1.04571400	2.09263500	-3.84821700
H -3.81748938	3.36251723	0.39255741	H 0.14961600	2.59078300	2.65290100
H -2.17812291	2.74166299	0.60490943	H 0.14961600	2.59078300	-2.65290100
H -3.43705345	2.36261481	1.78926143	C -1.65439300	-1.01948300	3.15787300
C -3.26551370	-1.60054908	-0.66658642	C -1.65439300	-1.01948300	-3.15787300
H -4.25258371	-1.68369496	-0.19905620	H -1.83179800	-1.89240100	2.51894900
C -3.43782313	-1.34502593	-2.16216550	H -1.83179800	-1.89240100	-2.51894900
H -2.47150106	-1.22152137	-2.65424698	C -2.83121500	-0.07149000	2.94624000
H -4.03859453	-0.45670463	-2.36830074	C -2.83121500	-0.07149000	-2.94624000
H -3.94209817	-2.19722803	-2.62727023	H -3.76655800	-0.58121200	3.19661700
C -2.50373260	-2.89886820	-0.41441330	H -3.76655800	-0.58121200	-3.19661700
H -3.00667254	-3.72719063	-0.92225798	H -2.88805000	0.25557800	1.90731600

H -2.45129698	-3.14803208	0.64734642	H -2.88805000	0.25557800	-1.90731600
H -1.48465478	-2.83727031	-0.80248767	H -2.76427700	0.81298200	3.58328800
C 3.60192378	1.34406215	-0.17278811	H -2.76427700	0.81298200	-3.58328800
H 4.58744620	0.99399941	0.15107757	C -1.54083100	-1.47733600	4.60866300
C 3.61949982	1.56139412	-1.68569033	C -1.54083100	-1.47733600	-4.60866300
H 2.63969993	1.88549424	-2.04253915	H -1.42446100	-0.63117700	5.29041400
H 3.89493167	0.65893051	-2.23551776	H -1.42446100	-0.63117700	-5.29041400
H 4.34628676	2.33796728	-1.94070608	H -0.70266200	-2.15972700	4.77231000
C 3.28932017	2.64330239	0.56391394	H -0.70266200	-2.15972700	-4.77231000
H 3.99292763	3.41713168	0.24317867	H -2.45344100	-2.00329200	4.90555400
H 3.38943094	2.54529913	1.64635234	H -2.45344100	-2.00329200	-4.90555400
H 2.28257038	2.99788239	0.34255052	C 1.00944300	-1.91012800	2.44677300
C 3.21845073	-1.56487520	-0.46561641	C 1.00944300	-1.91012800	-2.44677300
H 3.05383447	-1.45353930	-1.54230699	H 1.58948200	-1.96897700	3.36975000
C 2.48853921	-2.82973426	-0.01641898	H 1.58948200	-1.96897700	-3.36975000
H 2.82876342	-3.68464894	-0.60726916	H 0.33221900	-2.77018800	2.44006500
H 1.40812510	-2.74029727	-0.14559996	H 0.33221900	-2.77018800	-2.44006500
H 2.69325986	-3.05557651	1.03334592	C 1.93150500	-1.97660400	1.23709800
C 4.71734383	-1.67775504	-0.20148950	C 1.93150500	-1.97660400	-1.23709800
H 4.94085226	-1.69512160	0.86924264	H 2.68687400	-1.18906500	1.27910600
H 5.28806724	-0.86529994	-0.65353521	H 2.68687400	-1.18906500	-1.27910600
H 5.09547878	-2.61339142	-0.62434251	H 2.45454800	-2.94286600	1.21216100
N 0.00601888	2.09896012	-0.43251422	H 2.45454800	-2.94286600	-1.21216100
N -0.00585067	-0.48514699	1.78007077	N -1.18156700	1.63012100	0.00000000
O 0.00656930	3.14088572	-1.02895340	N 1.15461000	-1.78223300	0.00000000
P -2.42474436	-0.14821862	0.16807435	H 0.38653300	-2.44969200	0.00000000
P 2.40047023	-0.03080928	0.24766320	O -1.90629400	2.57061100	0.00000000
W -0.00697633	0.24194233	-0.14657835	O 2.54823400	1.89109100	0.00000000
C 0.15098743	-0.70228318	-1.85282502	P -0.06221000	-0.36790000	2.39355700
O 0.26847613	-1.28375547	-2.86724709	P -0.06221000	-0.36790000	-2.39355700
			W -0.10342200	0.17631500	0.00000000
			H -1.38901600	-1.11059400	0.00000000
2W-trans-Cs			2W-C1		
C -1.48710400	1.55006700	0.00000000	C 0.01642600	-1.95758200	-0.61425900
C 0.72038500	0.79153700	3.64078200	C 3.67783300	-1.01341600	-0.48126900
C 0.72038500	0.79153700	-3.64078200	C -3.63504100	-1.10551500	-0.47609400
H 0.59988000	0.31813900	4.62130500	H 3.48344300	-0.98168200	-1.55839000
H 0.59988000	0.31813900	-4.62130500	H -4.61454400	-0.81571100	-0.08431200
C 2.21112100	0.99579800	3.37752900	C 5.13880700	-0.64525000	-0.22981300
C 2.21112100	0.99579800	-3.37752900	C -3.35318900	-2.53310300	-0.02042900
H 2.38592500	1.43404300	2.39371100	H 5.35794000	-0.55628800	0.83895100
H 2.38592500	1.43404300	-2.39371100	H -2.38687200	-2.88905200	-0.37515500
H 2.78279700	0.06813000	3.45282700	H 5.43317600	0.28618800	-0.71403100
H 2.78279700	0.06813000	-3.45282700	H -3.38189600	-2.63721400	1.06707900
H 2.61916900	1.68498900	4.12304000	H 5.78619500	-1.43424700	-0.62439900
H 2.61916900	1.68498900	-4.12304000	H -4.12109300	-3.19950000	-0.42536300
C -0.00952900	2.13319700	3.63478200	C 3.40402600	-2.43708900	-0.00205100
C -0.00952900	2.13319700	-3.63478200	C -3.65328700	-1.00608000	-1.99995700
H 0.45366500	2.80986600	4.35916300	H 4.05412300	-3.13486500	-0.53763300
H 0.45366500	2.80986600	-4.35916300	H -4.36995700	-1.72049000	-2.41563800
H -1.06387900	2.03896600	3.89719600	H 2.37583100	-2.74547200	-0.17878100
H -1.06387900	2.03896600	-3.89719600	H -3.93846900	-0.01115100	-2.34982700
H 0.04901800	2.59851600	2.64885100	H 3.62655700	-2.55020200	1.06343700
H 0.04901800	2.59851600	-2.64885100	H -2.66804400	-1.23395400	-2.41342000
C -1.59460500	-1.08131800	3.19557400	C 3.26858200	1.85623100	-0.02752300
C -1.59460500	-1.08131800	-3.19557400	C -3.33201300	1.77340200	-0.03289300
H -1.75872600	-1.96873000	2.57321000	H 4.29402600	1.72562300	0.33056900
H -1.75872600	-1.96873000	-2.57321000	H -3.19463200	1.95636700	-1.10424400
C -2.81489300	-0.18369600	3.01858900	C 2.63165900	3.00184200	0.75034100
C -2.81489300	-0.18369600	-3.01858900	C -4.82881500	1.73116300	0.27185500
H -3.71586900	-0.72246400	3.32757200	H 3.15465700	3.93349300	0.51362300
H -3.71586900	-0.72246400	-3.32757200	H -5.25433300	2.73145200	0.14669200

H -2.93518600	0.11430500	1.97717900	H 2.69626000	2.86480900	1.83267200
H -2.93518600	0.11430500	-1.97717900	H -5.38112200	1.06323600	-0.38991200
H -2.75188900	0.71944500	3.62905500	H 1.57993200	3.11339200	0.48223800
H -2.75188900	0.71944500	-3.62905500	H -5.02441400	1.42642000	1.30451200
C -1.41401700	-1.51899900	4.64626100	C 3.29048600	2.17222200	-1.52352600
C -1.41401700	-1.51899900	-4.64626100	C -2.66768400	2.92641500	0.71433500
H -1.30252500	-0.66091500	5.31373400	H 2.27364500	2.27816500	-1.90802000
H -1.30252500	-0.66091500	-5.31373400	H -2.86779400	2.87595400	1.78946100
H -0.54804700	-2.17065700	4.78702300	H 3.78838200	1.39751000	-2.11101400
H -0.54804700	-2.17065700	-4.78702300	H -1.58823500	2.92809900	0.55954500
H -2.29721800	-2.07184700	4.98050600	H 3.82085400	3.11244800	-1.70052800
H -2.29721800	-2.07184700	-4.98050600	H -3.07485600	3.87736200	0.35909400
C 1.07917000	-1.89111600	2.45475100	C 2.46043600	-0.09272700	2.06432800
C 1.07917000	-1.89111600	-2.45475100	C -2.45574400	-0.14735800	2.06345300
H 1.67295800	-1.92222400	3.37070200	H 3.37951200	-0.60451600	2.35790900
H 1.67295800	-1.92222400	-3.37070200	H -3.36347400	-0.67638500	2.36165500
H 0.43465100	-2.77627700	2.46167700	H 2.46755800	0.88199900	2.55819500
H 0.43465100	-2.77627700	-2.46167700	H -2.48035200	0.83151100	2.55030600
C 1.98746500	-1.92883500	1.23409900	C 1.24628200	-0.89152000	2.52255800
C 1.98746500	-1.92883500	-1.23409900	C -1.22366800	-0.91737700	2.52361500
H 2.71667400	-1.11664500	1.26688800	H 1.28856300	-1.91350300	2.14055700
H 2.71667400	-1.11664500	-1.26688800	H -1.24269300	-1.94063900	2.14288100
H 2.54154400	-2.87760000	1.20241000	H 1.22172500	-0.94424600	3.62007000
H 2.54154400	-2.87760000	-1.20241000	H -1.19805800	-0.96758400	3.62120600
N 1.26189200	1.41386700	0.00000000	N -0.00905600	0.39201000	-2.06605100
N 1.19672600	-1.75577100	0.00000000	N 0.00447500	-0.28123500	2.01205800
H 0.45629400	-2.45442300	0.00000000	H -0.00528800	0.69787800	2.28885700
O 2.11734800	2.24798600	0.00000000	O -0.01772400	0.67067600	-3.21944400
O -2.33002400	2.34998500	0.00000000	O 0.03649800	-3.10677400	-0.82057900
P -0.04532800	-0.38109800	2.38948500	P 2.40381000	0.20145100	0.21199800
P -0.04532800	-0.38109800	-2.38948500	P -2.40647900	0.14033900	0.21095700
W -0.08116300	0.16877300	0.00000000	W 0.00098100	0.00770500	-0.29731100
H -1.42374500	-1.08955800	0.00000000	H 0.01251900	1.70560800	0.29999200
1Cr-cis + H₂-TS			1Cr-trans + H₂-TS		
C 1.30758500	1.23610500	0.00000000	N 1.01216000	1.34928800	0.00000000
O 2.21506800	1.95317900	0.00000000	O 1.76009600	2.26128200	0.00000000
Cr -0.11705400	0.08466600	0.00000000	Cr -0.06693700	0.08733300	0.00000000
P -0.05732700	-0.31500400	2.31922600	P -0.03660900	-0.33122000	2.32431700
P -0.05732700	-0.31500400	-2.31922600	P -0.03660900	-0.33122000	-2.32431700
C 0.97130200	-1.86174300	2.42353100	C 1.06403800	-1.82849500	2.43021300
C 0.97130200	-1.86174300	-2.42353100	C 1.06403800	-1.82849500	-2.43021300
H 0.26890700	-2.70001400	2.39499300	H 0.40440800	-2.70143300	2.41973800
H 0.26890700	-2.70001400	-2.39499300	H 0.40440800	-2.70143300	-2.41973800
H 1.53507800	-1.93326800	3.35555600	H 1.64479700	-1.86131400	3.35443300
H 1.53507800	-1.93326800	-3.35555600	H 1.64479700	-1.86131400	-3.35443300
C 1.87753000	-1.92434600	1.20167800	C 1.95109500	-1.85552700	1.19420400
C 1.87753000	-1.92434600	-1.20167800	C 1.95109500	-1.85552700	-1.19420400
H 2.34226000	-2.92400200	1.15690500	H 2.46890500	-2.82978700	1.15535900
H 2.34226000	-2.92400200	-1.15690500	H 2.46890500	-2.82978700	-1.15535900
H 2.71018200	-1.20717600	1.32435800	H 2.74632700	-1.09322900	1.29782100
H 2.71018200	-1.20717600	-1.32435800	H 2.74632700	-1.09322900	-1.29782100
N 1.12151900	-1.66846200	0.00000000	N 1.16877800	-1.65232000	0.00000000
C -1.66473300	-0.89393300	-3.11020000	C -1.59253900	-0.97931000	-3.16640700
C -1.66473300	-0.89393300	3.11020000	C -1.59253900	-0.97931000	3.16640700
H -1.93767100	-1.71374000	-2.43519100	H -1.84893800	-1.81722200	-2.50678500
H -1.93767100	-1.71374000	2.43519100	H -1.84893800	-1.81722200	2.50678500
C 0.68050100	0.90457000	-3.54473100	C 0.69078100	0.93398000	-3.50485200
C 0.68050100	0.90457000	3.54473100	C 0.69078100	0.93398000	3.50485200
C 2.20756900	0.92114100	-3.51198400	C 2.20754900	1.05017900	-3.36148700
C 2.20756900	0.92114100	3.51198400	C 2.20754900	1.05017900	3.36148700
N -1.24204300	1.31320900	0.00000000	C -1.50134900	1.24010700	0.00000000
O -2.01985200	2.19742100	0.00000000	O -2.37476100	1.99803800	0.00000000

H 0.36417500	0.56219200	4.53570400	H 0.46913900	0.56460400	4.51200700
H 0.36417500	0.56219200	-4.53570400	H 0.46913900	0.56460400	-4.51200700
C 0.12606600	2.30900000	3.30565000	C 0.03192400	2.30111100	3.32106400
C 0.12606600	2.30900000	-3.30565000	C 0.03192400	2.30111100	-3.32106400
H -0.96284900	2.34681800	3.34477600	H -1.05184800	2.26812300	3.43478300
H -0.96284900	2.34681800	-3.34477600	H -1.05184800	2.26812300	-3.43478300
H 0.43303700	2.68684500	2.32888700	H 0.25050600	2.70875900	2.33303400
H 0.43303700	2.68684500	-2.32888700	H 0.25050600	2.70875900	-2.33303400
H 0.51157900	2.99436100	4.06657300	H 0.42297100	3.00136700	4.06548900
H 0.51157900	2.99436100	-4.06657300	H 0.42297100	3.00136700	-4.06548900
C -2.78242300	0.14374000	-3.04782200	C -2.76661300	-0.00438600	-3.15103900
C -2.78242300	0.14374000	3.04782200	C -2.76661300	-0.00438600	3.15103900
H -2.61380500	0.95906900	-3.75524200	H -2.61400800	0.81889300	-3.85247800
H -2.61380500	0.95906900	3.75524200	H -2.61400800	0.81889300	3.85247800
H -2.88827600	0.57427000	-2.05199800	H -2.93993100	0.42059100	-2.16291600
H -2.88827600	0.57427000	2.05199800	H -2.93993100	0.42059100	2.16291600
H -3.73517400	-0.32189100	-3.31763400	H -3.67976500	-0.52225800	-3.45963800
H -3.73517400	-0.32189100	3.31763400	H -3.67976500	-0.52225800	3.45963800
C -1.51297400	-1.45957200	-4.52034600	C -1.35893400	-1.53044900	-4.57170700
C -1.51297400	-1.45957200	4.52034600	C -1.35893400	-1.53044900	4.57170700
H -0.73635000	-2.22432100	-4.58568600	H -0.54492100	-2.25659600	-4.60974400
H -0.73635000	-2.22432100	4.58568600	H -0.54492100	-2.25659600	4.60974400
H -1.27955400	-0.67677100	-5.24653300	H -1.13521700	-0.73258700	-5.28436600
H -1.27955400	-0.67677100	5.24653300	H -1.13521700	-0.73258700	5.28436600
H -2.45397200	-1.91884500	-4.83873900	H -2.26399700	-2.03199600	-4.92797400
H -2.45397200	-1.91884500	4.83873900	H -2.26399700	-2.03199600	4.92797400
H -1.22504200	-1.33630700	0.00000000	H -1.21526900	-1.34449500	0.00000000
H -0.37339400	-1.69807900	0.00000000	H -0.39484300	-1.69825800	0.00000000
H 2.57761500	1.63757200	-4.25168300	H 2.58242300	1.78640300	-4.07899300
H 2.58573800	1.23440400	-2.53774500	H 2.49071100	1.39110200	-2.36463800
H 2.64403700	-0.04970600	-3.75196100	H 2.72150000	0.10865400	-3.56096500
H 2.57761500	1.63757200	4.25168300	H 2.58242300	1.78640300	4.07899300
H 2.64403700	-0.04970600	3.75196100	H 2.72150000	0.10865400	3.56096500
H 2.58573800	1.23440400	2.53774500	H 2.49071100	1.39110200	2.36463800
2Cr-cis + PhCN-TS-H_M transfer			2Cr-trans + PhCN-TS-H_M transfer		
N -0.41861300	-1.83564600	0.00000000	N -2.44571300	-0.65732100	0.00000000
O -0.13395300	-2.98137100	0.00000000	O -3.56569300	-1.04686700	0.00000000
Cr -0.79321100	-0.22000200	0.00000000	Cr -0.85175500	-0.19229600	0.00000000
P -0.68884100	0.15100100	2.31876100	P -0.69468500	0.16598300	2.32251200
P -0.68884100	0.15100100	-2.31876100	P -0.69468500	0.16598300	-2.32251200
C -0.92170400	1.99774700	2.43316700	C -0.93958900	2.01284900	2.43795400
C -0.92170400	1.99774700	-2.43316700	C -0.93958900	2.01284900	-2.43795400
H 0.07835600	2.43921500	2.40615900	H 0.05673700	2.46329100	2.41955800
H 0.07835600	2.43921500	-2.40615900	H 0.05673700	2.46329100	-2.41955800
H -1.39551000	2.31167900	3.36465200	H -1.42556700	2.32288500	3.36479800
H -1.39551000	2.31167900	-3.36465200	H -1.42556700	2.32288500	-3.36479800
C -1.70534900	2.47844100	1.22346500	C -1.71690200	2.48286900	1.22014600
C -1.70534900	2.47844100	-1.22346500	C -1.71690200	2.48286900	-1.22014600
H -1.71860400	3.57691200	1.19570600	H -1.73726100	3.58130200	1.18903700
H -1.71860400	3.57691200	-1.19570600	H -1.73726100	3.58130200	-1.18903700
H -2.74255300	2.13688200	1.26282700	H -2.75207000	2.13472000	1.25432500
H -2.74255300	2.13688200	-1.26282700	H -2.75207000	2.13472000	-1.25432500
N -1.08406100	1.94578600	0.00000000	N -1.08927100	1.94889100	0.00000000
C 0.94522900	-0.07959400	-3.21963800	C 0.92562300	-0.04636100	-3.25388100
C 0.94522900	-0.07959400	3.21963800	C 0.92562300	-0.04636100	3.25388100
H 1.64152600	0.41299400	-2.53371900	H 1.62989400	0.45597700	-2.58284000
H 1.64152600	0.41299400	2.53371900	H 1.62989400	0.45597700	2.58284000
C -1.95076300	-0.60704400	-3.49828400	C -1.98974000	-0.58320900	-3.46560800
C -1.95076300	-0.60704400	3.49828400	C -1.98974000	-0.58320900	3.46560800
C -3.29233000	0.12293900	-3.50230100	C -3.34665900	0.11136500	-3.36183800
C -3.29233000	0.12293900	3.50230100	C -3.34665900	0.11136500	3.36183800
C -2.60445800	-0.49654700	0.00000000	C -0.23686100	-1.91235900	0.00000000

O -3.74412200	-0.71830000	0.00000000	O 0.14648100	-3.00604700	0.00000000
H -1.51352400	-0.52099100	4.49890200	H -1.60874400	-0.43899000	4.48261600
H -1.51352400	-0.52099100	-4.49890200	H -1.60874400	-0.43899000	-4.48261600
C -2.15671000	-2.08832100	3.17894200	C -2.14515700	-2.08225400	3.20549600
C -2.15671000	-2.08832100	-3.17894200	C -2.14515700	-2.08225400	-3.20549600
H -1.22447300	-2.65318000	3.16869400	H -1.20056700	-2.62303400	3.26344200
H -1.22447300	-2.65318000	-3.16869400	H -1.20056700	-2.62303400	-3.26344200
H -2.62612800	-2.21286000	2.20215400	H -2.57177600	-2.26248600	2.21815600
H -2.62612800	-2.21286000	-2.20215400	H -2.57177600	-2.26248600	-2.21815600
H -2.81417400	-2.54089700	3.92774700	H -2.82311900	-2.51568100	3.94738400
H -2.81417400	-2.54089700	-3.92774700	H -2.82311900	-2.51568100	-3.94738400
C 1.34743900	-1.54916900	-3.32087700	C 1.35515600	-1.50639200	-3.37693800
C 1.34743900	-1.54916900	3.32087700	C 1.35515600	-1.50639200	3.37693800
H 0.75263400	-2.07361700	-4.07304000	H 0.75696800	-2.03558000	-4.12275300
H 0.75263400	-2.07361700	4.07304000	H 0.75696800	-2.03558000	4.12275300
H 1.23456100	-2.07426900	-2.37149200	H 1.27444300	-2.04427600	-2.43206200
H 1.23456100	-2.07426900	2.37149200	H 1.27444300	-2.04427600	2.43206200
H 2.39501200	-1.62751600	-3.62537900	H 2.39770300	-1.55832400	-3.70342700
H 2.39501200	-1.62751600	3.62537900	H 2.39770300	-1.55832400	3.70342700
C 1.03804000	0.60832000	-4.57959600	C 0.97578500	0.64989000	-4.61229400
C 1.03804000	0.60832000	4.57959600	C 0.97578500	0.64989000	4.61229400
H 0.81578100	1.67568400	-4.52769000	H 0.73600200	1.71264600	-4.55081100
H 0.81578100	1.67568400	4.52769000	H 0.73600200	1.71264600	4.55081100
H 0.36376900	0.15689400	-5.31226100	H 0.29339100	0.18888100	-5.33123500
H 0.36376900	0.15689400	5.31226100	H 0.29339100	0.18888100	5.33123500
H 2.05344200	0.50599100	-4.97487700	H 1.98384000	0.56682300	-5.02993600
H 2.05344200	0.50599100	4.97487700	H 1.98384000	0.56682300	5.02993600
H 0.85287700	0.32717700	0.00000000	H 0.88448300	0.25946700	0.00000000
H -0.10252300	2.28175700	0.00000000	H -0.10425900	2.28547000	0.00000000
N 1.71744900	2.59737400	0.00000000	N 1.69210700	2.51619400	0.00000000
C 2.09425500	1.47920700	0.00000000	C 2.05224000	1.38786300	0.00000000
C 3.25940600	0.60003100	0.00000000	C 3.25876500	0.55792800	0.00000000
C 3.16953500	-0.78789700	0.00000000	C 3.23403100	-0.83191400	0.00000000
C 4.32362900	-1.55966800	0.00000000	C 4.42137100	-1.55221400	0.00000000
C 5.57199000	-0.95130800	0.00000000	C 5.64095900	-0.88871000	0.00000000
C 4.51918300	1.21342500	0.00000000	C 4.49042600	1.22602100	0.00000000
C 5.66631000	0.43734700	0.00000000	C 5.67149000	0.50295400	0.00000000
H 2.18530600	-1.23996500	0.00000000	H 2.27703900	-1.33595900	0.00000000
H 4.24423800	-2.64086500	0.00000000	H 4.38998100	-2.63589500	0.00000000
H 6.47204200	-1.55624600	0.00000000	H 6.56738800	-1.45238300	0.00000000
H 4.57791700	2.29523700	0.00000000	H 4.49875700	2.30935200	0.00000000
H 6.63881700	0.91692700	0.00000000	H 6.62122300	1.02631500	0.00000000
H -3.96998900	-0.36721400	-4.20799300	H -4.04875700	-0.36171300	-4.05516400
H -3.77006000	0.08964800	-2.52165800	H -3.76826100	0.01616500	-2.35980300
H -3.20533200	1.16634100	-3.81074300	H -3.30028900	1.17024600	-3.62273200
H -3.96998900	-0.36721400	4.20799300	H -4.04875700	-0.36171300	4.05516400
H -3.20533200	1.16634100	3.81074300	H -3.30028900	1.17024600	3.62273200
H -3.77006000	0.08964800	2.52165800	H -3.76826100	0.01616500	2.35980300
2Cr-cis + PhCN-interm			2Cr-trans + PhCN-interm		
N -0.41939300	-1.82910000	0.00000000	N -0.00624800	2.43799300	-0.63471700
O -0.16696900	-2.97978700	0.00000000	O -0.00921100	3.57132300	-0.97538700
Cr -0.78191300	-0.20621300	0.00000000	Cr -0.00221400	0.84876500	-0.18735900
P -0.68526200	0.15229700	2.33935000	P -2.33942100	0.68063800	0.16557100
P -0.68526200	0.15229700	-2.33935000	P 2.33557000	0.69200100	0.16549500
C -0.84977000	2.00273900	2.43908900	C -2.44328400	0.86856100	2.01624500
C -0.84977000	2.00273900	-2.43908900	C 2.43812700	0.87818600	2.01643800
H 0.16736800	2.40272700	2.41525800	H -2.42230500	-0.14203800	2.43286400
H 0.16736800	2.40272700	-2.41525800	H 2.42132200	-0.13306100	2.43170700
H -1.31999300	2.34175500	3.36355300	H -3.36751300	1.34649400	2.34582300
H -1.31999300	2.34175500	-3.36355300	H 3.36032900	1.35948800	2.34680500
C -1.59925800	2.50169200	1.21526200	C -1.21913800	1.62524100	2.50322100
C -1.59925800	2.50169200	-1.21526200	C 1.21082900	1.62910600	2.50437600

H -1.54224700	3.59797400	1.16890800	H -1.17482700	1.58972400	3.60064600
H -1.54224700	3.59797400	-1.16890800	H 1.16644900	1.59146200	3.60172900
H -2.65800000	2.23173800	1.26010900	H -1.26217500	2.67803500	2.21148300
H -2.65800000	2.23173800	-1.26010900	H 1.24962400	2.68260700	2.21458900
N -1.00283700	1.91886200	0.00000000	N -0.00292500	1.02281600	1.92985000
C 0.93882400	-0.14266000	-3.23861500	C 3.26616100	-0.92028000	-0.10141000
C 0.93882400	-0.14266000	3.23861500	C -3.26042400	-0.93727200	-0.09976200
H 1.65744800	0.32534400	-2.55816200	H 2.59892800	-1.64323600	0.37934800
H 1.65744800	0.32534400	2.55816200	H -2.58883900	-1.65583200	0.38149600
C -1.98314100	-0.56787300	-3.49911800	C 3.46410200	2.01669700	-0.54914500
C -1.98314100	-0.56787300	3.49911800	C -3.47502100	1.99800300	-0.55129900
C -3.29974500	0.20638200	-3.48816800	C 3.35228500	3.35106800	0.18660100
C -3.29974500	0.20638200	3.48816800	C -3.37076500	3.33388400	0.18285700
C -2.57473800	-0.48716700	0.00000000	C -0.00079100	0.26419400	-1.92747300
O -3.71650300	-0.69082300	0.00000000	O 0.00025800	-0.06548500	-3.03670100
H -1.55191100	-0.49132400	4.50304500	H -4.49170900	1.61266500	-0.41716900
H -1.55191100	-0.49132400	-4.50304500	H 4.48284300	1.63685900	-0.41504900
C -2.23092600	-2.04358300	3.18404400	C -3.21614400	2.19368800	-2.04571100
C -2.23092600	-2.04358300	-3.18404400	C 3.20486100	2.21276400	-2.04342900
H -1.31539800	-2.63502800	3.17751600	H -3.27376700	1.26390000	-2.61142200
H -1.31539800	-2.63502800	-3.17751600	H 3.26732700	1.28384900	-2.61006300
H -2.70461600	-2.15932900	2.20840500	H -2.23019600	2.62723300	-2.21662500
H -2.70461600	-2.15932900	-2.20840500	H 2.21683900	2.64157900	-2.21420200
H -2.90147700	-2.47363000	3.93429000	H -3.95967700	2.88172500	-2.45969600
H -2.90147700	-2.47363000	-3.93429000	H 3.94510600	2.90493800	-2.45640600
C 1.28825400	-1.62536100	-3.34517800	C 3.39206100	-1.30320100	-1.57408100
C 1.28825400	-1.62536100	3.34517800	C -3.38421500	-1.32205500	-1.57212700
H 0.67165000	-2.12728600	-4.09509000	H 4.13578500	-0.68619000	-2.08423300
H 0.67165000	-2.12728600	4.09509000	H -4.13275400	-0.71085100	-2.08222700
H 1.16598900	-2.15011100	-2.39679400	H 2.44739600	-1.21202800	-2.11073100
H 1.16598900	-2.15011100	2.39679400	H -2.44052200	-1.22414400	-2.10928200
H 2.33063300	-1.73715800	-3.65607900	H 3.72251300	-2.34229300	-1.65656900
H 2.33063300	-1.73715800	3.65607900	H -3.70698800	-2.36360900	-1.65384200
C 1.04883500	0.54519200	-4.59767800	C 4.62387700	-0.98652500	0.59522600
C 1.04883500	0.54519200	4.59767800	C -4.61776800	-1.01135700	0.59695200
H 0.86697800	1.61980600	-4.54155700	H 4.55937900	-0.78165600	1.66498000
H 0.86697800	1.61980600	4.54155700	H -4.55453500	-0.80655000	1.66680900
H 0.35511300	0.12012600	-5.32798800	H 5.34099900	-0.28737300	0.15697600
H 0.35511300	0.12012600	5.32798800	H -5.33883500	-0.31612000	0.15894500
H 2.05811700	0.40649900	-4.99686500	H 5.04429700	-1.99013300	0.48071000
H 2.05811700	0.40649900	4.99686500	H -5.03251000	-2.01728900	0.48212000
H 1.00950900	0.40557400	0.00000000	H 0.00317300	-1.00857900	0.35667700
H 0.03645000	2.25444000	0.00000000	H -0.00121500	-0.00611600	2.25513900
N 1.63415300	2.45660800	0.00000000	N 0.00255900	-1.64337900	2.42620200
C 1.90920600	1.26932300	0.00000000	C 0.00441800	-1.91987000	1.24277100
C 3.19743900	0.53332900	0.00000000	C 0.00823400	-3.21232200	0.51273900
C 3.23592100	-0.85743900	0.00000000	C 0.00877000	-3.27223700	-0.87662800
C 4.45257200	-1.52870700	0.00000000	C 0.01233400	-4.49859700	-1.53033200
C 5.64115200	-0.81037100	0.00000000	C 0.01542600	-5.67677500	-0.79563400
C 4.39599100	1.25241000	0.00000000	C 0.01131000	-4.40147600	1.24841300
C 5.60848000	0.58223500	0.00000000	C 0.01489600	-5.62349200	0.59625500
H 2.30131100	-1.40884000	0.00000000	H 0.00634100	-2.34904500	-1.44454800
H 4.47151400	-2.61307700	0.00000000	H 0.01270600	-4.53223800	-2.61430800
H 6.59214500	-1.33184100	0.00000000	H 0.01823200	-6.63511500	-1.30340600
H 4.34711800	2.33535500	0.00000000	H 0.01079500	-4.33722000	2.33045100
H 6.53557600	1.14543300	0.00000000	H 0.01730000	-6.54192900	1.17342800
H -3.99887400	-0.25863800	-4.18972500	H 4.04254600	4.07053600	-0.26411200
H -3.77014300	0.18603200	-2.50371000	H 2.34838200	3.77069700	0.10398000
H -3.17993100	1.24723300	-3.79354300	H 3.61204300	3.27299700	1.24371100
H -3.99887400	-0.25863800	4.18972500	H -4.06456900	4.04912700	-0.26913700
H -3.17993100	1.24723300	3.79354300	H -3.63070400	3.25578800	1.23992900
H -3.77014300	0.18603200	2.50371000	H -2.36903500	3.75869100	0.10028300
2Cr-cis + PhCN-TS-H_N transfer			2Cr-trans + PhCN-TS-H_N transfer		

Cr -0.19932700	-0.80897400	0.00000000	N 0.60245600	-2.47507300	0.00000000
N 1.89552900	-0.91586800	0.00000000	O 0.89674800	-3.62052500	0.00000000
H 0.31201200	1.08932000	0.00000000	Cr 0.18014700	-0.88374500	0.00000000
H 2.21594400	0.25391900	0.00000000	P -0.15943500	-0.70868100	2.34416200
C 1.15996100	1.93365500	0.00000000	P -0.15943500	-0.70868100	-2.34416200
N 2.35264900	1.62705700	0.00000000	C -2.01565200	-0.75537600	2.44650300
C 0.49993100	3.25939400	0.00000000	C -2.01565200	-0.75537600	-2.44650300
C -0.88877900	3.36437400	0.00000000	H -2.35366000	0.28397500	2.45415300
C -1.50106400	4.61165000	0.00000000	H -2.35366000	0.28397500	-2.45415300
C -0.72596300	5.76408100	0.00000000	H -2.37945300	-1.23072800	3.35933300
C 0.66360600	5.66520900	0.00000000	H -2.37945300	-1.23072800	-3.35933300
C 1.27503100	4.42221000	0.00000000	C -2.55241400	-1.44185900	1.20151300
P 0.14659000	-0.70239400	-2.34323900	C -2.55241400	-1.44185900	-1.20151300
P 0.14659000	-0.70239400	2.34323900	H -3.63887100	-1.28093900	1.13989700
N -1.83308500	-0.48649700	0.00000000	H -3.63887100	-1.28093900	-1.13989700
C -0.42914200	-2.60302900	0.00000000	H -2.39370600	-2.52488600	1.25361400
C -0.23692300	0.90517400	3.24062700	H -2.39370600	-2.52488600	-1.25361400
C -0.23692300	0.90517400	-3.24062700	N -1.89830400	-0.90147700	0.00000000
C -0.50642200	-2.04019800	3.49612900	C 0.22583900	0.88206900	-3.27326800
C -0.50642200	-2.04019800	-3.49612900	C 0.22583900	0.88206900	3.27326800
O -0.58429100	-3.75205600	0.00000000	H -0.22765100	1.63316700	-2.61748900
C 2.00094200	-0.76588300	-2.44418400	H -0.22765100	1.63316700	2.61748900
C 2.00094200	-0.76588300	2.44418400	C 0.45561600	-2.08716800	-3.46465100
H 2.34388000	0.27186300	-2.44130200	C 0.45561600	-2.08716800	3.46465100
H 2.34388000	0.27186300	2.44130200	C -0.35703300	-3.37224300	-3.31289300
H 2.36419500	-1.23362900	-3.36073600	C -0.35703300	-3.37224300	3.31289300
H 2.36419500	-1.23362900	3.36073600	C 1.93293100	-0.32344400	0.00000000
C 2.53701000	-1.46498600	-1.20548900	O 3.04802500	-0.01447400	0.00000000
C 2.53701000	-1.46498600	1.20548900	H 0.31987500	-1.71609300	4.48642000
H 3.62492200	-1.31580700	-1.14704500	H 0.31987500	-1.71609300	-4.48642000
H 3.62492200	-1.31580700	1.14704500	C 1.94139300	-2.36630700	3.23524200
H 2.36586700	-2.54568500	-1.25923200	C 1.94139300	-2.36630700	-3.23524200
H 2.36586700	-2.54568500	1.25923200	H 2.55998100	-1.47471000	3.33611400
H 0.21670600	1.64414800	2.57192500	H 2.55998100	-1.47471000	-3.33611400
H 0.21670600	1.64414800	-2.57192500	H 2.11212900	-2.78007600	2.24089000
C 0.32852400	-3.31896700	3.46671700	H 2.11212900	-2.78007600	-2.24089000
C 0.32852400	-3.31896700	-3.46671700	H 2.29376500	-3.09997300	3.96675300
O -2.99019600	-0.26369400	0.00000000	H 2.29376500	-3.09997300	-3.96675300
H -0.44112200	-1.61469700	-4.50321200	C 1.71870500	1.18613100	-3.37182600
H -0.44112200	-1.61469700	4.50321200	C 1.71870500	1.18613100	3.37182600
C -1.97184400	-2.35214100	-3.19051200	H 2.20917900	0.54300900	-4.10637100
C -1.97184400	-2.35214100	3.19051200	H 2.20917900	0.54300900	4.10637100
H -2.60455400	-1.46466500	-3.19993500	H 2.23312400	1.06693600	-2.41820300
H -2.60455400	-1.46466500	3.19993500	H 2.23312400	1.06693600	2.41820300
H -2.07506600	-2.81966600	-2.21053600	H 1.86198000	2.21905000	-3.70129600
H -2.07506600	-2.81966600	2.21053600	H 1.86198000	2.21905000	3.70129600
H -2.36386600	-3.05010600	-3.93656600	C -0.44066300	0.98404100	-4.64412900
H -2.36386600	-3.05010600	3.93656600	C -0.44066300	0.98404100	4.64412900
C -1.73353200	1.19806400	3.31773300	H -1.52015400	0.83069200	-4.60115300
C -1.73353200	1.19806400	-3.31773300	H -1.52015400	0.83069200	4.60115300
H -2.22750400	0.55915000	4.05399200	H -0.02225100	0.26489600	-5.35315600
H -2.22750400	0.55915000	-4.05399200	H -0.02225100	0.26489600	5.35315600
H -2.23390600	1.06097600	2.35830700	H -0.26935600	1.98118000	-5.06067200
H -2.23390600	1.06097600	-2.35830700	H -0.26935600	1.98118000	5.06067200
H -1.89088500	2.23365900	3.63201200	H -0.26695300	1.11179200	0.00000000
H -1.89088500	2.23365900	-3.63201200	H -2.20078900	0.29839700	0.00000000
C 0.41972500	1.03878000	4.61301000	N -2.30865700	1.64265700	0.00000000
C 0.41972500	1.03878000	-4.61301000	C -1.11570600	1.95314800	0.00000000
H 1.50035300	0.88970200	4.57888700	C -0.47509600	3.28854400	0.00000000
H 1.50035300	0.88970200	-4.57888700	C 0.91129300	3.42032700	0.00000000
H 0.00131700	0.33296100	5.33540900	C 1.50024400	4.67891700	0.00000000
H 0.00131700	0.33296100	-5.33540900	C 0.70414300	5.81671600	0.00000000

H 0.24167400	2.04366300	5.00769500	C -1.27109500	4.43753800	0.00000000
H 0.24167400	2.04366300	-5.00769500	C -0.68328000	5.69169000	0.00000000
H -1.48756800	2.45886800	0.00000000	H 1.53012700	2.52917600	0.00000000
H -2.58319400	4.68319600	0.00000000	H 2.58086600	4.77009400	0.00000000
H -1.20125600	6.73894600	0.00000000	H 1.16125000	6.80021500	0.00000000
H 2.35441000	4.32136400	0.00000000	H -2.34835800	4.31661000	0.00000000
H 1.26990900	6.56465900	0.00000000	H -1.30652600	6.57946300	0.00000000
H -0.09775800	-4.04528800	-4.16528100	H 0.03325200	-4.12909600	-3.99998300
H -0.09775800	-4.04528800	4.16528100	H -0.27874600	-3.77905700	-2.30356600
H 1.36489600	-3.15264800	-3.76514500	H -1.41284800	-3.23247700	-3.55052000
H 1.36489600	-3.15264800	3.76514500	H 0.03325200	-4.12909600	3.99998300
H 0.32329100	-3.78058200	-2.47808900	H -1.41284800	-3.23247700	3.55052000
H 0.32329100	-3.78058200	2.47808900	H -0.27874600	-3.77905700	2.30356600
2Cr-cis + PhCHNH-TS			2Cr-trans + PhCHNH-TS		
Cr -0.55495000	0.49939700	-0.21481000	N -0.67835100	0.68485100	1.94303000
N -0.66367300	0.67579400	1.94834200	H 0.53325600	-0.86881400	0.25445500
H 0.52058400	-0.83127300	0.28626600	H -0.07559700	-0.13195800	2.26597900
H -0.03544000	-0.11150800	2.27145800	C 0.96708100	-1.90753200	1.21627200
C 1.02341100	-1.91176700	1.29609500	N 0.97357400	-1.47178100	2.47262400
N 1.08225600	-1.43457200	2.52568300	C 2.19338500	-2.41138900	0.50283000
C 2.20818700	-2.41712300	0.52539900	C 2.13481300	-2.75806500	-0.84799000
C 2.10821800	-2.69296600	-0.83944800	C 3.23821800	-3.29171500	-1.49566800
C 3.17643300	-3.23837500	-1.53414700	C 4.42714400	-3.49117700	-0.80084700
C 4.36975800	-3.51824200	-0.87485400	C 4.49518500	-3.16017100	0.54536700
C 4.47928700	-3.25373200	0.48323500	C 3.38392500	-2.63163200	1.19321800
C 3.40305300	-2.71432700	1.17939200	P -2.46776600	-0.87649500	0.15616300
P -2.42333800	-0.90593300	0.13827900	P 1.37996500	1.80318300	0.13156800
P 1.36030500	1.82696900	0.11915900	C 3.09107800	1.07595500	-0.13507600
N -0.35949000	0.20919600	-1.83769200	C -2.47664400	-2.73164800	-0.18265800
C -1.61168300	1.96821900	-0.45476200	C 1.49961400	3.54017500	-0.58563300
C 3.05980700	1.07936500	-0.15542500	C -4.15132600	-0.31281900	-0.47406000
C -2.35075500	-2.74641500	-0.26358000	O -2.10662600	2.75111700	-1.09823200
C 1.51572300	3.54860400	0.63803800	C -2.60163400	-0.83930600	2.01500700
C -4.14287000	-0.43003300	-0.47990500	C 1.36509600	2.03866700	1.98200900
O -2.26954300	2.90547500	-0.64885800	H -2.00180600	-1.67248600	2.39330100
C -2.53065600	-0.91063800	1.99818400	H 1.97282700	1.23320400	2.40315000
C 1.34389700	2.07199100	1.96748700	H -3.62413900	-0.97755000	2.37256300
H -1.89100600	-1.72567000	2.34949200	H 1.81230500	2.98331100	2.29694300
H 1.96739400	1.27835900	2.38767900	C -2.01169500	0.46440900	2.52766900
H -3.53930900	-1.10211300	2.36913000	C -0.06039100	1.90434500	2.48949600
H 1.77654500	3.02423900	2.27808500	H -1.94199800	0.43193700	3.62402300
C -1.98742200	0.40515600	2.53301300	H -0.06287200	1.87126400	3.58849600
C -0.07569300	1.91336900	2.48648700	H -2.64959900	1.31220500	2.26528800
H -1.91253900	0.35773400	3.62825300	H -0.66389500	2.76442200	2.18773300
H -0.07045900	1.88390300	3.58536200	H 2.99285100	0.09626900	0.34336200
H -2.65549500	1.23426900	2.28592800	H -1.53575300	-3.05313300	0.27429400
H -0.69939200	2.75908300	2.18532100	C 0.61500200	4.55135500	0.14227800
H 2.95402400	0.10416800	0.33010500	C -4.72079100	0.86767600	0.31078200
H -1.36785300	-3.03267700	0.12103300	O 0.03786800	-0.38325400	-2.96938500
C 0.74949100	4.62781400	0.12429500	H -4.81700600	-1.16927800	-0.32295800
C -4.83875200	0.61852300	0.38561700	H 2.54408500	3.83978400	-0.44559200
O -0.21390000	-0.01390000	-2.98560500	C -4.10745200	0.01386800	-1.96784200
H -4.73257700	-1.35146100	-0.42991600	C 1.18608600	3.54318600	-2.08287000
H 2.58233700	3.79248800	-0.58913200	H -3.69417500	-0.79704600	-2.56713600
C -4.09150500	0.03396400	-1.93658000	H 1.78712900	2.82673800	-2.64240500
C 1.08838800	3.52980000	-2.10646300	H -3.51117600	0.90635400	-2.15681700
H -3.58849800	-0.67760800	-2.59107000	H 0.13605600	3.31133100	-2.26256300
H 1.60548500	2.76611900	-2.68749700	H -5.12226900	0.20888800	-2.32848100
H -3.57076100	0.98749400	-2.02571400	H 1.38330200	4.53729800	-2.49615800
H 0.01772100	3.34394700	-2.19874400	C 3.41620500	0.83431500	-1.60726200
H -5.10925800	0.17343700	-2.31419700	C -2.40250400	-3.07300900	-1.66948500
H 1.30025000	4.50052300	-2.56541100	H 3.63392000	1.77051700	-2.12724100

C	3.34426600	0.82610100	-1.63397000	H	-3.35971000	-2.90100600	-2.16670600
C	-2.34511500	-3.01205200	-1.76783400	H	2.60599900	0.32854600	-2.13244600
H	3.54559700	1.75843500	-2.16797300	H	-1.63954700	-2.49470100	-2.19195800
H	-3.33225400	-2.84706100	-2.20611200	H	4.30612300	0.20419100	-1.68617900
H	2.51579400	0.31759300	-2.12850900	H	-2.16372300	-4.13342300	-1.79286300
H	-1.62788400	-2.38230900	-2.29689700	C	4.22223200	1.83832400	0.55209900
H	4.23083500	0.19453200	-1.73592800	C	-3.60545800	-3.50065700	0.50109300
H	-2.08011400	-4.05630900	-1.95775400	H	4.05108100	1.97977500	1.62078200
C	4.21295100	1.83066400	0.50565600	H	-3.64109400	-3.32589800	1.57767000
C	-3.39725100	-3.60359600	0.44490500	H	4.38236000	2.82185700	0.10251300
H	4.05943300	1.98488700	1.57558800	H	-4.58292000	-3.24787100	0.08274000
H	-3.37101600	-3.48624500	1.52970100	H	5.15722500	1.28071600	0.44243700
H	4.38135200	2.80780700	0.04511300	H	-3.46156000	-4.57480300	0.34929400
H	-4.41077700	-3.37740100	0.10379800	H	1.21654400	-2.58675500	-1.39878700
H	5.13822400	1.25848000	0.38788900	H	3.17277700	-3.54969000	-2.54704100
H	-3.21580900	-4.66054600	0.22646300	H	5.29131100	-3.90874900	-1.30563300
H	1.18932400	-2.44481600	-1.35950000	H	3.43528500	-2.41807200	2.25518500
H	3.08173000	-3.44033200	-2.59552300	H	5.41140500	-3.32837300	1.10114400
H	5.20640300	-3.94400500	-1.41778900	H	-5.70309100	1.12878000	-0.09463600
H	3.48175500	-2.55185700	2.24885100	H	0.74768200	5.53851100	-0.31096900
H	5.39983700	-3.48218300	1.00953100	H	-4.85882700	0.64089700	1.36952900
H	-5.83220000	0.82403800	-0.02467300	H	0.86561600	4.64677700	1.20035900
H	0.89292500	5.59231800	-0.37241300	H	-4.08859800	1.75217300	0.22078400
H	-4.97763000	0.28995900	1.41717600	H	-0.44190000	4.29520900	0.05504900
H	1.09257800	4.74244600	1.15408800	H	0.10015300	-2.52049500	0.96764600
H	-4.29250200	1.56305100	0.39180400	H	1.89821500	-1.12013400	2.72019100
H	-0.32317100	4.42873400	0.13630100	Cr	-0.58223400	0.53083000	-0.19321600
H	0.12871200	-2.49567100	1.08433600	C	-0.19959300	-0.02867900	-1.89353900
H	2.01827300	-1.07942400	2.72270900	N	-1.48679700	1.82682400	-0.68813300
2Cr-cis + PhCHNCH₂Ph-TS				2Cr-trans + PhCHNCH₂Ph-TS			
O	-3.26142200	0.41844800	1.97517800	O	-2.53866900	-0.05760800	2.77520000
Cr	-1.43141300	-0.25137200	-0.08884600	Cr	-1.32449400	0.59626900	0.12322200
P	-1.40424600	1.79817500	-1.23873400	P	0.26237000	2.16081400	0.91062800
P	-0.91056000	-2.45637000	0.68841600	P	-2.47346300	-1.06407100	-1.13082000
C	0.12372500	1.59177700	-2.28397900	C	1.38156500	2.32734700	-0.57221800
C	0.42159000	-2.98565500	-0.50150400	C	-1.40566400	-1.14327100	-2.66074700
H	0.95893400	1.94819500	-1.67653200	H	2.20936200	1.62833700	-0.43699000
H	1.37103300	-2.76718400	-0.00609000	H	-0.64201000	-1.90641100	-2.48505900
H	0.10377700	2.19560600	-3.19379000	H	1.81666200	3.32363200	-0.66764700
H	0.39463500	-4.05207500	-0.72987600	H	-1.96160900	-1.44047800	-3.55246000
C	0.31933800	0.12155100	-2.61738700	C	0.60929000	1.94394100	-1.82351400
C	0.33427100	-2.15093500	-1.76720300	C	-0.72745700	0.20297800	-2.86491000
H	1.29605400	-0.03000900	-3.09668800	H	1.29623100	1.88884600	-2.67898400
H	1.23352200	-2.31110900	-2.37737500	H	0.00570100	0.12920300	-3.68001000
H	-0.44299100	-0.20859900	-3.32826800	H	-0.15193900	2.69252900	-2.05759100
H	-0.53091100	-2.43491400	-2.37194200	H	-1.45772200	0.96341600	-3.15123000
N	0.21017700	-0.72320400	-1.41495900	N	-0.06542700	0.64800200	-1.62595800
C	-0.05169500	-2.79865600	2.33402400	C	-2.59670700	-2.87887100	-0.62536400
C	-1.01386600	3.36191600	-0.27735300	C	1.48134600	1.76739100	2.29001300
H	0.85471600	-2.19310700	2.23952500	H	-1.59096800	-3.10152600	-0.25926800
H	-0.15811800	3.03081600	0.31681700	H	1.77695800	0.74299200	2.04422500
C	-2.24027500	-3.79531200	0.63205500	C	-4.21132200	-0.69491000	-1.76302900
C	-2.74929400	2.34168600	-2.44496500	C	-0.28701600	3.91944500	1.31308000
C	-2.47698500	-4.37729100	-0.76013300	C	-4.24057500	0.32148500	-2.90324400
C	-2.71920300	1.58929000	-3.77397100	C	-0.58215000	4.76290700	0.07338000
O	-3.57163700	-1.28198000	-1.89038900	O	-3.24277000	2.61534600	-0.44323400
C	-4.13538300	2.23967700	-1.80623200	C	-1.49265100	3.92665700	2.25498500
C	-3.54796600	-3.28334100	1.23639900	C	-5.13695500	-0.24323200	-0.63123400
H	-4.20124400	2.76489200	-0.85364600	H	-1.33573100	3.32551300	3.15003600
H	-3.41610100	-2.87236600	2.23807400	H	-5.13272500	-0.92395800	0.21911600
H	-4.41101600	1.19953600	-1.63091400	H	-2.38397500	3.55150300	1.75233600
H	-3.98816400	-2.50114600	0.61715500	H	-4.85908900	0.74599300	-0.26899300

H -4.88312900	2.67320300	-2.47759100	H -1.69838800	4.95265400	2.57603600
H -4.27010700	-4.10282600	1.30439400	H -6.16431900	-0.18453500	-1.00427400
C -0.85238800	-2.28176300	3.52651400	C -3.55336800	-3.10427100	0.54442800
C -2.11488800	3.75387300	0.70547600	C 0.82555600	1.73868800	3.66914200
H -1.72650100	-2.90721600	3.72307200	H -4.59656500	-3.02438200	0.23071100
H -2.97373500	4.19604300	0.19483600	H 0.60797600	2.74750600	4.02770400
H -1.20264800	-1.25949100	3.37239600	H -3.38287200	-2.40158100	1.36102700
H -2.46246900	2.90476400	1.29446000	H -0.10399200	1.16771500	3.67856500
H -0.23591900	-2.29999900	4.43051200	H -3.41290800	-4.11403200	0.94057200
H -1.73110800	4.50627100	1.40041500	H 1.50761000	1.27987600	4.39060200
C 0.39793700	-4.24279100	2.54766800	C -2.90023300	-3.83869600	-1.77407500
C -0.58254900	4.55468800	-1.12662900	C 2.73197500	2.64367900	2.30447200
H 0.96370700	-4.63538400	1.70018400	H -2.17890000	-3.76135100	-2.58932100
H 0.23192900	4.31367800	-1.81323300	H 3.27421500	2.62198800	1.35782300
H -0.44488600	-4.91260600	2.73396300	H -3.89865400	-3.67736000	-2.18862000
H -1.41048000	4.95956400	-1.71446100	H 2.49557700	3.68587300	2.53463600
H 1.04742600	-4.29764100	3.42689800	H -2.86938400	-4.86938400	-1.40772100
H -0.23240500	5.36024800	-0.47390000	H 3.41730200	2.29248000	3.08204800
H -0.03176800	0.57640300	0.72763200	H -0.07469600	-0.68004000	0.59877800
H 1.02689700	-0.52103700	-0.77866800	H 0.68580500	-0.05443700	-1.41675400
N 2.20483300	-0.13454100	0.51579100	N 1.79185900	-1.35557700	-0.73014400
H -2.53735600	3.39612900	-2.65172100	H 0.56456000	4.37182300	1.83354900
H -1.86058800	-4.60183400	1.26596300	H -4.57973300	-1.64947600	-2.15439500
H -3.23802100	-5.16124600	-0.69686000	H -5.27474200	0.46220200	-3.23204100
H -3.51243300	1.97114200	-4.42401400	H -0.86737700	5.77220900	0.38562700
H -2.84495000	-3.62696500	-1.45982200	H -3.86954900	1.29563500	-2.58131600
H -2.90106700	0.52223100	-3.63802000	H -1.41562900	4.35527700	-0.50027300
H -1.57979200	-4.83408500	-1.18171000	H -3.66752400	-0.00328600	-3.77357700
H -1.77612700	1.71669100	-4.30884400	H 0.28164500	4.86279100	-0.58602100
C 3.23481200	0.65672800	-0.10858600	C 3.07281000	-0.96737600	-0.18923200
H 2.85016100	1.39644400	-0.83267800	H 2.98435300	-0.17249100	0.56962600
H 3.79325600	1.24857900	0.63443900	H 3.54688800	-1.80250500	1.34893800
C 4.23410600	-0.20632500	-0.84887300	C 4.03812300	-0.49731200	-1.25345800
C 4.52969200	-1.49773500	-0.41822800	C 3.84302400	-0.79624400	-2.59938000
C 4.91591200	0.29753700	-1.95566200	C 5.17754300	0.22234100	-0.89010400
C 5.48482100	-2.26360700	-1.07508300	C 4.76362800	-0.38635400	-3.55784200
H 3.99196900	-1.88910900	0.43717500	H 2.95768300	-1.35537500	-2.87694800
C 5.87191000	-0.46484900	-2.61556500	C 6.09816800	0.63323700	-1.84438800
H 4.69454700	1.30147900	-2.30771600	H 5.34655100	0.46178500	0.15624500
C 6.16036500	-1.75110400	-2.17642700	C 5.89389300	0.32980700	-3.18596500
H 5.70461000	-3.26683000	-0.72475300	H 4.59733900	-0.63062200	-4.60200700
H 6.38947600	-0.05509000	-3.47644700	H 6.97693600	1.19246800	-1.54119000
H 6.90463300	-2.34991300	-2.68988900	H 6.61095500	0.64990500	-3.93394700
C 1.33777900	0.39123900	1.37851900	C 0.86874700	-1.79521900	0.10863900
H 0.89068500	-0.34402000	2.03902900	H 0.04004100	-2.27828700	-0.40427400
C 1.47479600	1.68640300	2.12719700	C 1.18349200	-2.48393100	1.41458300
C 1.08018700	1.68857700	3.46840300	C 1.91245800	-3.67675000	1.34266200
C 1.98673400	2.87593000	1.59965800	C 0.75401800	-2.04466500	2.66197800
C 1.20296100	2.82101100	4.25934400	C 2.20908500	-4.39928000	2.48902600
H 0.67057400	0.77988100	3.89721900	H 2.24530800	-4.03578900	0.37426000
C 2.11293100	4.01271600	2.38900400	C 1.04845100	-2.76906800	3.81247800
H 2.28316200	2.93034500	0.56146900	H 0.17714300	-1.13134600	2.72633600
C 1.72576800	3.99072300	3.72211800	C 1.77801800	-3.94647100	3.73127100
H 0.89059500	2.78994000	5.29741200	H 2.77495100	-5.32151800	2.41203500
H 2.51774200	4.92128100	1.95637600	H 0.70020000	-2.40984600	4.77481500
H 1.82763800	4.87835000	4.33647600	H 2.00833600	-4.51066900	4.62827700
N -2.51176100	0.14666900	1.10958200	N -2.43357400	1.77247000	-0.23748400
C -2.71013200	-0.91833800	-1.20102500	C -2.06701600	0.19248100	1.74888100
2Cr-cis + PhCHNPh-TS			2Cr-trans + PhCHNPh-TS		
O -1.93751200	0.16733200	2.97596800	O -1.58675700	0.06356600	3.14593000
Cr -1.23018300	0.47784200	0.24501200	P 0.20664300	2.30538200	0.33511000
P 0.26193200	2.27755300	0.48012800	P -2.44198300	-1.48574500	-0.52152200

P	-2.45754100	-1.37256100	-0.59323400	C	0.92568800	2.31142300	-1.38421700
C	0.98048400	2.39584100	-1.23450100	C	-1.92732700	-1.58460100	-2.31318400
C	-1.85638900	-1.43651500	-2.35873800	H	1.82524400	1.69106200	-1.35744800
H	1.86810100	1.75793700	-1.24805200	H	-1.05629100	-2.24457600	-2.36124200
H	-0.97334600	-2.08249600	-2.37334700	H	1.22877100	3.30770000	-1.71274900
H	1.30445200	3.40553700	-1.49223200	H	-2.70317000	-2.00935600	-2.95409100
H	-2.58714500	-1.87015900	-3.04371400	C	-0.07885100	1.70502100	-2.34906200
C	-0.03188600	1.87349500	-2.24236800	C	-1.52542800	-0.19778700	-2.78981400
C	-1.45013600	-0.03895900	-2.80355600	H	0.38456600	1.57530600	-3.33668700
H	0.42946500	1.81195600	-3.23752100	H	-1.07638900	-0.26390700	-3.79068100
H	-0.97775300	-0.08678600	-3.79444800	H	-0.94167400	2.36380800	-2.47530200
H	-0.88998200	2.54621300	-2.31937500	H	-2.39562500	0.45861700	-2.86354300
H	-2.32197300	0.61426200	-2.88689700	N	-0.57354700	0.41176900	-1.84400900
N	-0.52019300	0.54770700	-1.82430500	C	-2.07785500	-3.25000000	0.05700200
C	-2.16862100	-3.13748200	0.01196800	C	1.75069300	2.25565400	1.40664000
C	1.78506900	2.06450800	1.55602700	H	-1.07561100	-3.42075100	-0.34921900
H	-1.08015300	-3.20103000	0.09006200	H	2.10768800	1.23922800	1.21867000
H	2.11109100	1.06318400	1.26355800	C	-4.32268800	-1.42460600	-0.58607200
C	-4.34429300	-1.31315500	-0.69325800	C	-0.45293500	4.05348600	0.58470200
C	-0.32467300	4.01802800	0.91926100	C	-4.86352400	-0.43866700	-1.62014200
C	-4.88059600	-0.51785300	-1.88175800	C	-1.18780600	4.59843900	-0.63915700
C	-0.91397400	4.78984900	-0.25986000	O	-3.56121900	2.15194200	0.13616500
O	-3.47903000	2.35768200	-0.33448000	C	-1.34761100	4.14926600	1.82218400
C	-1.31977300	3.98144800	2.08044600	C	-4.90987400	-1.14527200	0.79672200
C	-4.94807300	-0.78941000	0.61112700	H	-0.87265700	3.75801300	2.72104900
H	-0.94347300	3.43276900	2.94366000	H	-4.59161800	-1.87697600	1.54088000
H	-4.57720800	-1.31365400	1.49150100	H	-2.28130700	3.60714100	1.67319400
H	-2.25774500	3.51546200	1.77764800	H	-4.62311400	-0.15600100	1.15526100
H	-4.73350700	0.27061200	0.74521500	H	-1.59859700	5.19804600	2.00993900
H	-1.54443700	5.00211800	2.40553800	H	-6.00251000	-1.17953100	0.74765200
H	-6.03581800	-0.90791500	0.58507300	C	-1.98586800	-3.37010000	1.57566600
C	-2.72833000	-3.35832900	1.41639100	C	1.45285000	2.36850400	2.90036200
C	1.44344400	2.02406300	3.04393600	H	-2.95876800	-3.23904100	2.05389900
H	-3.81960900	-3.41057800	1.40980100	H	1.21218700	3.39595700	3.18283800
H	1.19452300	3.01769500	3.42471900	H	-1.30491500	-2.63256200	2.00032200
H	-2.42585200	-2.57133700	2.10925900	H	0.62842800	1.72654500	3.21252000
H	0.60776500	1.35653100	3.25889200	H	-1.61997800	-4.36420000	1.84891700
H	-2.36241900	-4.31015000	1.81194000	H	2.33832900	2.07668100	3.47224000
H	2.30936000	1.66960800	3.61050000	C	-2.98364300	-4.32635500	-0.53766200
C	-2.63277000	-4.23075300	-0.94777300	C	2.84312600	3.24005500	0.99606000
C	2.91582800	3.05037700	1.27642400	H	-3.07953800	-4.24337300	-1.62287400
H	-2.17942400	-4.14083100	-1.93656400	H	3.14763600	3.12108200	-0.04463200
H	3.23538500	3.03705400	0.23330600	H	-3.98565500	-4.29975600	-0.10322700
H	-3.71874300	-4.23373500	-1.07220900	H	2.53307000	4.27777000	1.14529600
H	2.63827100	4.07528000	1.53712500	H	-2.56717400	-5.31465000	-0.32086500
H	-2.35450500	-5.21128800	-0.54927500	H	3.73088200	3.08079300	1.61598800
H	3.78701800	2.79222100	1.88655100	H	0.29537800	-0.42742200	0.48348600
H	0.27383300	-0.47204800	0.35897700	H	0.23398300	-0.23952000	-1.78427200
H	0.30588400	-0.08144300	-1.79922200	N	1.61492900	-1.45320900	-1.32974300
N	1.75509600	-1.25906700	-1.48738200	H	0.43677200	4.67232100	0.74696700
H	0.57494900	4.54757200	1.25088600	H	-4.62962900	-2.42680100	-0.89901600
H	-4.65407600	-2.35554800	-0.82215000	H	-5.95662500	-0.49237300	-1.62470100
H	-5.97417600	-0.55746500	-1.87734100	H	-1.52256600	5.61979200	-0.43350900
H	-1.20618500	5.79047000	0.07328000	H	-4.59050100	0.59025800	-1.38856800
H	-4.59806100	0.53424700	-1.82433700	H	-2.07616800	4.00783800	-0.86837700
H	-1.81102200	4.30720800	-0.65051700	H	-4.52800100	-0.67222900	-2.63246200
H	-4.54820900	-0.91609800	-2.84205100	H	-0.55480400	4.63972800	-1.52735500
H	-0.20349000	4.91810000	-1.07834500	C	1.24821100	-1.66277800	-0.07954300
C	1.26056400	-1.67396800	-0.34201000	H	0.34874800	-2.26274600	-0.00061100
H	0.32725800	-2.21125000	-0.46763100	C	2.15767100	-1.91735700	1.09072300
C	2.01082100	-2.16537000	0.86111300	C	3.26205100	-2.75370200	0.89846500
C	3.10429100	-3.01418900	0.66273500	C	1.86545800	-1.48830300	2.38362600
C	1.56952600	-1.93645500	2.16339100	C	4.05988000	-3.13088400	1.96877100

C 3.74802500	-3.60192800	1.74207100	H 3.49230300	-3.10832200	-0.09925600
H 3.44727600	-3.21234900	-0.34610600	C 2.66575500	-1.86480900	3.45554800
C 2.21538200	-2.52531200	3.24357600	H 1.00836400	-0.84737100	2.54564800
H 0.71969100	-1.28248900	2.31859100	C 3.76763800	-2.68487400	3.25252400
C 3.30847100	-3.35702600	3.03798000	H 4.91250400	-3.77932000	1.79860000
H 4.59529600	-4.25660200	1.56904600	H 2.42224900	-1.51587900	4.45317400
H 1.86090900	-2.33053300	4.24996200	H 4.39300900	-2.97806600	4.08853500
H 3.81406900	-3.81417300	3.88145600	C 2.82627600	-0.88662200	-1.71837800
C 3.01529700	-0.68982200	-1.66132600	C 3.16619000	-1.04412200	-3.07446200
C 3.45920200	-0.59363100	-2.99230100	C 3.71151000	-0.14425700	-0.91661100
C 3.85982400	-0.17608300	-0.66213400	C 4.33113300	-0.51019600	-3.59777900
C 4.68453700	-0.03328700	-3.30994400	H 2.48597000	-1.61141900	-3.70019300
H 2.80981100	-0.98481800	-3.76768100	C 4.87569700	0.39468700	-1.44863300
C 5.08546600	0.39038400	-0.98700900	H 3.49579000	0.00056400	0.13288600
H 3.56434300	-0.23323900	0.37612500	C 5.19881600	0.21678900	-2.78790900
C 5.51072600	0.46577700	-2.30736700	H 4.56460100	-0.65992400	-4.64678100
H 4.99805600	0.01677400	-4.34745900	H 5.54029000	0.95910100	-0.80257800
H 5.71721700	0.77494800	-0.19298700	H 6.11086000	0.63814700	-3.19492000
H 6.47013800	0.90710000	-2.55203400	C -1.46210700	0.21669000	2.00573400
C -2.60747800	1.61593000	-0.13722800	N -2.61593400	1.43592500	0.10727600
N -1.64844300	0.30549200	1.84187900	Cr -1.26865400	0.47384300	0.20580600
2Cr-cis + PhCCH-TS			2Cr-trans + PhCCH-TS		
N 1.17976200	-2.35462000	0.00000000	O 2.45267300	-2.83114100	0.00000000
O 1.99149200	-3.20996000	0.00000000	P -0.01747000	-0.71939100	2.31118900
P 0.00112900	-0.74102100	2.30432800	P -0.01747000	-0.71939100	-2.31118900
P 0.00112900	-0.74102100	-2.30432800	C -1.18074700	0.73988900	2.44576500
C -1.10718700	0.75738800	2.43926200	C -1.18074700	0.73988900	-2.44576500
C -1.10718700	0.75738800	-2.43926200	H -0.56029300	1.64036100	2.46614100
H -0.45202000	1.63286800	2.44495600	H -0.56029300	1.64036100	-2.46614100
H -0.45202000	1.63286800	-2.44495600	H -1.77066300	0.73196400	3.36425200
H -1.68384200	0.77817700	3.36556400	H -1.77066300	0.73196400	-3.36425200
H -1.68384200	0.77817700	-3.36556400	C -2.07853600	0.77634700	1.22185300
C -2.02029300	0.82183300	1.22639800	C -2.07853600	0.77634700	-1.22185300
C -2.02029300	0.82183300	-1.22639800	H -2.64790900	1.71564700	1.19579900
H -2.55500900	1.78124000	1.20347000	H -2.64790900	1.71564700	-1.19579900
H -2.55500900	1.78124000	-1.20347000	H -2.79532000	-0.04753000	1.23941300
H -2.76708100	0.02513700	1.25633000	H -2.79532000	-0.04753000	-1.23941300
H -2.76708100	0.02513700	-1.25633000	N -1.26745200	0.63131900	0.00000000
N -1.22394500	0.64789700	0.00000000	C 1.48139900	-0.03261500	-3.22074400
C 1.56083600	-0.09892200	-3.13885600	C 1.48139900	-0.03261500	3.22074400
C 1.56083600	-0.09892200	3.13885600	H 1.72218600	0.83141800	-2.59152400
H 1.77070900	0.77779300	-2.51656700	H 1.72218600	0.83141800	2.59152400
H 1.77070900	0.77779300	2.51656700	C -0.74004000	-2.01270700	-3.47036800
C -0.70908900	-1.98767900	-3.52525500	C -0.74004000	-2.01270700	3.47036800
C -0.70908900	-1.98767900	3.52525500	C -2.25020400	-2.16886200	-3.29981600
C -2.23225100	-2.08100100	-3.46287400	C -2.25020400	-2.16886200	3.29981600
C -2.23225100	-2.08100100	3.46287400	O -1.74844400	-3.36277700	0.00000000
C -1.37808000	-2.28349000	0.00000000	H -0.54521600	-1.65355100	4.48656800
O -2.23567900	-3.06775300	0.00000000	H -0.54521600	-1.65355100	-4.48656800
H -0.43060200	-1.63038600	4.52201900	C -0.04316600	-3.35969900	3.27677900
H -0.43060200	-1.63038600	-4.52201900	C -0.04316600	-3.35969900	-3.27677900
C -0.08353600	-3.36395500	3.29857600	H 1.03741500	-3.29904000	3.40884500
C -0.08353600	-3.36395500	-3.29857600	H 1.03741500	-3.29904000	-3.40884500
H 1.00435400	-3.35065400	3.37192300	H -0.23525200	-3.75550100	2.27857300
H 1.00435400	-3.35065400	-3.37192300	H -0.23525200	-3.75550100	-2.27857300
H -0.34157900	-3.74868600	2.31032300	H -0.42680100	-4.08169100	4.00425300
H -0.34157900	-3.74868600	-2.31032300	H -0.42680100	-4.08169100	-4.00425300
H -0.45911400	-4.07134600	4.04425300	C 2.68990400	-0.96477000	-3.20251400
H -0.45911400	-4.07134600	-4.04425300	C 2.68990400	-0.96477000	3.20251400
C 2.74517100	-1.05122200	-2.99731800	H 2.55431300	-1.81413000	-3.87599800
C 2.74517100	-1.05122200	2.99731800	H 2.55431300	-1.81413000	3.87599800
H 2.64265200	-1.92552800	-3.64431400	H 2.89693800	-1.35337100	-2.20582900

H 2.64265200	-1.92552800	3.64431400	H 2.89693800	-1.35337100	2.20582900
H 2.86229500	-1.40148500	-1.97131200	H 3.57719000	-0.42348200	-3.54486500
H 2.86229500	-1.40148500	1.97131200	H 3.57719000	-0.42348200	3.54486500
H 3.66815900	-0.54168300	-3.29080900	C 1.19597300	0.46397500	-4.63648800
H 3.66815900	-0.54168300	3.29080900	C 1.19597300	0.46397500	4.63648800
C 1.38507400	0.36331700	-4.58301300	H 0.34930800	1.15201900	-4.68209000
C 1.38507400	0.36331700	4.58301300	H 0.34930800	1.15201900	4.68209000
H 0.54348300	1.04886000	-4.70748000	H 0.99633900	-0.36273800	-5.32292000
H 0.54348300	1.04886000	4.70748000	H 0.99633900	-0.36273800	5.32292000
H 1.23791600	-0.47870400	-5.26406100	H 2.07033300	0.99603500	-5.02396400
H 1.23791600	-0.47870400	5.26406100	H 2.07033300	0.99603500	5.02396400
H 2.28588600	0.88836600	-4.91583700	H 1.24351600	0.14595600	0.00000000
H 2.28588600	0.88836600	4.91583700	H -0.57042600	1.38280400	0.00000000
H 1.19817800	0.16787400	0.00000000	C 1.98990700	1.55080600	0.00000000
H -0.49877800	1.37264500	0.00000000	H -2.61636500	-2.92909800	-3.99651800
C 1.97042700	1.60742100	0.00000000	H -2.50596800	-2.50123900	-2.29266100
H -2.58067300	-2.81407800	-4.19683900	H -2.79574800	-1.24757200	-3.51375500
H -2.57478100	-2.41632000	-2.48298000	H -2.61636500	-2.92909800	3.99651800
H -2.72342300	-1.13434100	-3.69672800	H -2.79574800	-1.24757200	3.51375500
H -2.58067300	-2.81407800	4.19683900	H -2.50596800	-2.50123900	2.29266100
H -2.72342300	-1.13434100	3.69672800	C 1.39954300	2.63841500	0.00000000
H -2.57478100	-2.41632000	2.48298000	C 0.61911800	3.80948300	0.00000000
C 1.36854000	2.68637000	0.00000000	C 0.22797500	4.42632900	1.20752500
C 0.60008200	3.86733800	0.00000000	C 0.22797500	4.42632900	-1.20752500
C 0.21533600	4.48697800	1.20715100	C -0.52988300	5.58449500	1.19956000
C 0.21533600	4.48697800	-1.20715100	H 0.54252600	3.98924700	2.14809800
C -0.53015100	5.65337700	1.19953300	C -0.52988300	5.58449500	-1.19956000
H 0.52391600	4.04559900	2.14768900	H 0.54252600	3.98924700	-2.14809800
C -0.53015100	5.65337700	-1.19953300	C -0.92024000	6.17212800	0.00000000
H 0.52391600	4.04559900	-2.14768900	H -0.81436400	6.03919900	2.14256200
C -0.91396600	6.24494200	0.00000000	H -0.81436400	6.03919900	-2.14256200
H -0.81028800	6.11074200	2.14252200	H -1.51157000	7.08021400	0.00000000
H -0.81028800	6.11074200	-2.14252200	H 2.95673500	1.08483800	0.00000000
H -1.49581300	7.15916800	0.00000000	Cr 0.01017300	-1.12075100	0.00000000
H 2.92797700	1.12583200	0.00000000	C 1.49723700	-2.17485300	0.00000000
Cr 0.05027100	-1.13808700	0.00000000	N -1.06439700	-2.39147100	0.00000000
2Cr-cis + PhCCH-TS-H_M transfer to Ph-C			2Cr-trans + PhCCH-TS-H_M transfer to Ph-C		
N -0.37592200	-1.82186600	0.00000000	O -0.15165400	-3.00032200	0.00000000
O -0.07026300	-2.96284600	0.00000000	Cr 0.86058500	-0.19043200	0.00000000
Cr -0.79234800	-0.21538900	0.00000000	P 0.68970200	0.16000600	-2.31657200
P -0.68339900	0.14670000	2.31614400	P 0.68970200	0.16000600	2.31657200
P -0.68339900	0.14670000	-2.31614400	C 0.94776200	2.00551400	-2.43671500
C -0.93756000	1.99072600	2.43259500	C 0.94776200	2.00551400	2.43671500
C -0.93756000	1.99072600	-2.43259500	H -0.04819700	2.45732800	-2.41560800
H 0.06059900	2.43712000	2.40302900	H -0.04819700	2.45732800	2.41560800
H 0.06059900	2.43712000	-2.40302900	H 1.43175400	2.31362300	-3.36522000
H -1.41170500	2.30213400	3.36477200	H 1.43175400	2.31362300	3.36522000
H -1.41170500	2.30213400	-3.36477200	C 1.72954400	2.47387900	-1.22134100
C -1.72625600	2.46496600	1.22391900	C 1.72954400	2.47387900	1.22134100
C -1.72625600	2.46496600	-1.22391900	H 1.74845900	3.57291300	-1.18525400
H -1.74266300	3.56403800	1.19029900	H 1.74845900	3.57291300	1.18525400
H -1.74266300	3.56403800	-1.19029900	H 2.76540100	2.12899300	-1.26106000
H -2.76285600	2.12278900	1.26799100	H 2.76540100	2.12899300	1.26106000
H -2.76285600	2.12278900	-1.26799100	N 1.11060500	1.93240700	0.00000000
N -1.11024900	1.92731400	0.00000000	C -0.93708400	-0.03976500	3.23798500
C 0.95622400	-0.06330200	-3.21072400	C -0.93708400	-0.03976500	-3.23798500
C 0.95622400	-0.06330200	3.21072400	H -1.63279300	0.46159300	2.55725900
H 1.64400200	0.43031000	-2.51684100	H -1.63279300	0.46159300	-2.55725900
H 1.64400200	0.43031000	2.51684100	C 1.97356200	-0.59759700	3.46732800
C -1.93355600	-0.62480500	-3.49975200	C 1.97356200	-0.59759700	-3.46732800
C -1.93355600	-0.62480500	3.49975200	C 3.33531300	0.08833100	3.36990400
C -3.28361700	0.08921400	-3.50382000	C 3.33531300	0.08833100	-3.36990400

C -3.28361700	0.08921400	3.50382000	O 3.57367000	-1.05357400	0.00000000
C -2.59443600	-0.52831700	0.00000000	H 1.58872200	-0.45287400	-4.48293400
O -3.73080900	-0.77014300	0.00000000	H 1.58872200	-0.45287400	4.48293400
H -1.49600800	-0.53296800	4.49981100	C 2.12104000	-2.09700500	-3.20470600
H -1.49600800	-0.53296800	-4.49981100	C 2.12104000	-2.09700500	3.20470600
C -2.12234300	-2.10854700	3.18112600	H 1.17281500	-2.63187800	-3.25765000
C -2.12234300	-2.10854700	-3.18112600	H 1.17281500	-2.63187800	3.25765000
H -1.18348200	-2.66225200	3.17205700	H 2.54980900	-2.27715500	-2.21823500
H -1.18348200	-2.66225200	-3.17205700	H 2.54980900	-2.27715500	2.21823500
H -2.58913000	-2.23882000	2.20379800	H 2.79361600	-2.53644500	-3.94802700
H -2.58913000	-2.23882000	-2.20379800	H 2.79361600	-2.53644500	3.94802700
H -2.77523300	-2.56837500	3.92958000	C -1.37293400	-1.49755900	3.36559700
H -2.77523300	-2.56837500	-3.92958000	C -1.37293400	-1.49755900	-3.36559700
C 1.37098400	-1.52884800	-3.32064000	H -0.78215800	-2.02551500	4.11837300
C 1.37098400	-1.52884800	3.32064000	H -0.78215800	-2.02551500	-4.11837300
H 0.78435600	-2.05304400	-4.07957800	H -1.28890000	-2.04000500	2.42377300
H 0.78435600	-2.05304400	4.07957800	H -1.28890000	-2.04000500	-2.42377300
H 1.25985000	-2.06145900	-2.37542300	H -2.41817500	-1.54327400	3.68413300
H 1.25985000	-2.06145900	2.37542300	H -2.41817500	-1.54327400	-3.68413300
H 2.42081700	-1.59530900	-3.61982600	C -0.99349000	0.66187600	4.59335200
H 2.42081700	-1.59530900	3.61982600	C -0.99349000	0.66187600	-4.59335200
C 1.04858600	0.63290800	-4.56649700	H -0.74877800	1.72357600	4.53039300
C 1.04858600	0.63290800	4.56649700	H -0.74877800	1.72357600	-4.53039300
H 0.81781100	1.69838600	-4.51040300	H -0.31789000	0.20095200	5.31889500
H 0.81781100	1.69838600	4.51040300	H -0.31789000	0.20095200	-5.31889500
H 0.38064000	0.18037900	-5.30443300	H -2.00477100	0.58450200	5.00434500
H 0.38064000	0.18037900	5.30443300	H -2.00477100	0.58450200	-5.00434500
H 2.06635600	0.54062500	-4.95818400	H -0.86361900	0.35339600	0.00000000
H 2.06635600	0.54062500	4.95818400	H 0.11533600	2.25453500	0.00000000
H 0.84001500	0.42851900	0.00000000	C -2.09891900	1.48327800	0.00000000
H -0.11870700	2.25160900	0.00000000	C -3.24768600	0.58509100	0.00000000
C 2.10473400	1.55057900	0.00000000	C -3.16229000	-0.80447800	0.00000000
C 3.22446100	0.61854400	0.00000000	C -4.30924400	-1.58777900	0.00000000
C 3.09042200	-0.76795500	0.00000000	C -5.56388700	-0.99449200	0.00000000
C 4.21131500	-1.58792000	0.00000000	C -4.52167100	1.17636100	0.00000000
C 5.48511400	-1.03626300	0.00000000	C -5.66385300	0.39399600	0.00000000
C 4.51656800	1.16817500	0.00000000	H -2.18182500	-1.25958200	0.00000000
C 5.63210500	0.34796600	0.00000000	H -4.21682800	-2.66824000	0.00000000
H 2.09137200	-1.18498800	0.00000000	H -6.45917400	-1.60637800	0.00000000
H 4.08386200	-2.66481200	0.00000000	H -4.59541300	2.25761800	0.00000000
H 6.35949400	-1.67775900	0.00000000	H -6.63881100	0.86939500	0.00000000
H 4.62571400	2.24648100	0.00000000	H 4.03269900	-0.39110800	4.06368800
H 6.62254800	0.79016800	0.00000000	H 3.75880300	-0.00682200	2.36855700
H -3.95613400	-0.40890200	-4.20890200	H 3.29514700	1.14684700	3.63385600
H -3.76012900	0.05054900	-2.52269000	H 4.03269900	-0.39110800	-4.06368800
H -3.20899000	1.13356000	-3.81276200	H 3.29514700	1.14684700	-3.63385600
H -3.95613400	-0.40890200	4.20890200	H 3.75880300	-0.00682200	-2.36855700
H -3.20899000	1.13356000	3.81276200	C -1.73414900	2.66784600	0.00000000
H -3.76012900	0.05054900	2.52269000	H -1.79846200	3.73346700	0.00000000
C 1.74841500	2.73490900	0.00000000	C 0.22740100	-1.90486800	0.00000000
H 1.74785600	3.80133500	0.00000000	N 2.45049200	-0.67029300	0.00000000
2Cr-cis + PhCCH-interm			2Cr-trans + PhCCH-interm		
N -0.37193500	-1.81118100	0.00000000	N -2.41949700	-0.68964300	0.00000000
O -0.07347500	-2.95116500	0.00000000	O -3.54244900	-1.06256300	0.00000000
Cr -0.79128100	-0.19975300	0.00000000	P -0.67958300	0.17156600	2.33753900
P -0.68394800	0.15906400	2.31975100	P -0.67958300	0.17156600	-2.33753900
P -0.68394800	0.15906400	-2.31975100	C -0.99050700	2.00879400	2.43701600
C -0.93804400	2.00011000	2.43234300	C -0.99050700	2.00879400	-2.43701600
C -0.93804300	2.00011000	-2.43234300	H -0.00764600	2.48842300	2.40417000
H 0.06069300	2.44470600	2.39181100	H -0.00764600	2.48842300	-2.40417000
H 0.06069300	2.44470600	-2.39181100	H -1.47407700	2.31211900	3.36698200
H -1.40923900	2.30888800	3.36680900	H -1.47407700	2.31211900	-3.36698200

H -1.40923900	2.30888800	-3.36680900	C -1.79824200	2.44386200	1.22626900
C -1.72471300	2.47402900	1.22222500	C -1.79824200	2.44386200	-1.22626900
C -1.72471300	2.47402900	-1.22222500	H -1.85882600	3.54025600	1.18637500
H -1.72800500	3.57240000	1.18529900	H -1.85882600	3.54025600	-1.18637500
H -1.72800500	3.57240000	-1.18529900	H -2.81906200	2.05852900	1.26979200
H -2.76592500	2.14453900	1.26767100	H -2.81906200	2.05852900	-1.26979200
H -2.76592500	2.14453900	-1.26767100	N -1.16326200	1.92432400	0.00000000
N -1.09998100	1.93099600	0.00000000	C 0.95709600	0.01427800	-3.24634700
C 0.95841100	-0.05457900	-3.21047600	C 0.95709600	0.01427800	3.24634700
C 0.95841100	-0.05457900	3.21047600	H 1.64206100	0.52351700	-2.56025100
H 1.64907000	0.44145300	-2.52065500	H 1.64206100	0.52351700	2.56025100
H 1.64907000	0.44145300	2.52065500	C -1.94384300	-0.62558700	-3.48040400
C -1.93425400	-0.61573400	-3.49805400	C -1.94384300	-0.62558700	3.48040400
C -1.93425400	-0.61573400	3.49805400	C -3.32056100	0.03192400	-3.40146300
C -3.28386700	0.09925600	-3.50410100	C -3.32056100	0.03192400	3.40146300
C -3.28386700	0.09925600	3.50410100	C -0.23095300	-1.92005400	0.00000000
C -2.58672900	-0.52644500	0.00000000	O 0.08429200	-3.03169500	0.00000000
O -3.72391100	-0.75778200	0.00000000	H -1.55243700	-0.48013300	4.49319700
H -1.49276700	-0.52137000	4.49584800	H -1.55243700	-0.48013300	-4.49319700
H -1.49276700	-0.52137000	-4.49584800	C -2.05760600	-2.12607700	3.20818700
C -2.12260200	-2.09887400	3.18093400	C -2.05760600	-2.12607700	-3.20818700
C -2.12260200	-2.09887400	-3.18093400	H -1.09530400	-2.63667700	3.24030700
H -1.18391800	-2.65293700	3.17366100	H -1.09530400	-2.63667700	-3.24030700
H -1.18391800	-2.65293700	-3.17366100	H -2.50134400	-2.31205500	2.22937000
H -2.58864700	-2.22870400	2.20335900	H -2.50134400	-2.31205500	-2.22937000
H -2.58864700	-2.22870400	-2.20335900	H -2.70454200	-2.58710700	3.96072500
H -2.77700100	-2.55834500	3.92799300	H -2.70454200	-2.58710700	-3.96072500
H -2.77700100	-2.55834500	-3.92799300	C 1.41848500	-1.43409500	-3.38924900
C 1.37051000	-1.51984700	-3.32130400	C 1.41848500	-1.43409500	3.38924900
C 1.37051000	-1.51984700	3.32130400	H 0.83552800	-1.96719100	-4.14459900
H 0.78355900	-2.04257900	-4.08086800	H 0.83552800	-1.96719100	4.14459900
H 0.78355900	-2.04257900	4.08086800	H 1.35358400	-1.98643400	-2.45152300
H 1.25958900	-2.05311300	-2.37648200	H 1.35358400	-1.98643400	2.45152300
H 1.25958900	-2.05311300	2.37648200	H 2.46315500	-1.45401900	-3.71042700
H 2.42049400	-1.58751800	-3.61845400	H 2.46315500	-1.45401900	3.71042700
H 2.42049400	-1.58751800	3.61845400	C 0.99817000	0.73338800	-4.59316100
C 1.04702800	0.64356900	-4.56582900	C 0.99817000	0.73338800	4.59316100
C 1.04702800	0.64356900	4.56582900	H 0.74165800	1.79113400	-4.51595200
H 0.81766800	1.70881500	-4.50643100	H 0.74165800	1.79113400	4.51595200
H 0.81766800	1.70881500	4.50643100	H 0.32842800	0.27202000	-5.32397900
H 0.37854900	0.19202800	-5.30393700	H 0.32842800	0.27202000	5.32397900
H 0.37854900	0.19202800	5.30393700	H 2.01027200	0.67504400	-5.00403100
H 2.06468800	0.55096200	-4.95724900	H 2.01027200	0.67504400	5.00403100
H 2.06468800	0.55096200	4.95724900	H 1.02820700	0.65444700	0.00000000
H 1.11701800	0.72916500	0.00000000	H -0.19332200	2.28516000	0.00000000
H -0.07683400	2.34607100	0.00000000	C 1.97934200	1.39506000	0.00000000
C 2.04105500	1.50064300	0.00000000	C 3.20251800	0.56103700	0.00000000
C 3.23044200	0.63446500	0.00000000	C 3.14904800	-0.83126000	0.00000000
C 3.09522800	-0.75510000	0.00000000	C 4.30787300	-1.59949700	0.00000000
C 4.21166400	-1.57924800	0.00000000	C 5.55119800	-0.98387400	0.00000000
C 5.48576100	-1.02578000	0.00000000	C 4.46533800	1.17058300	0.00000000
C 4.51650400	1.18001600	0.00000000	C 5.62034600	0.40819700	0.00000000
C 5.63177500	0.35885600	0.00000000	H 2.18032500	-1.31630600	0.00000000
H 2.09680000	-1.17953600	0.00000000	H 4.23452700	-2.68193200	0.00000000
H 4.08605600	-2.65670000	0.00000000	H 6.45832500	-1.57840100	0.00000000
H 6.36035900	-1.66697000	0.00000000	H 4.49991700	2.25426900	0.00000000
H 4.62438200	2.25949700	0.00000000	H 6.58694600	0.90152100	0.00000000
H 6.62345800	0.79895400	0.00000000	H -3.99890800	-0.46703700	-4.09995200
H -3.95440700	-0.39912800	-4.21071100	H -3.75467200	-0.06587900	-2.40489900
H -3.76316700	0.06010500	-2.52457900	H -3.30046400	1.08907100	-3.67232500
H -3.20898700	1.14360200	-3.81160000	H -3.99890800	-0.46703700	4.09995200
H -3.95440700	-0.39912800	4.21071100	H -3.30046400	1.08907100	3.67232500
H -3.20898700	1.14360200	3.81160000	H -3.75467200	-0.06587900	2.40489900

H -3.76316700	0.06010500	2.52457900	C 1.93333800	2.70030200	0.00000000
C 1.69474100	2.74859700	0.00000000	H 1.08074300	3.37848400	0.00000000
H 2.10931900	3.74542200	0.00000000	Cr -0.84927500	-0.18670400	0.00000000
2Cr-cis + PhCCH-TS-H_N transfer to C-H			2Cr-trans + PhCCH-TS-H_N transfer to C-H		
Cr -0.77128900	-0.20274400	0.00000000	N 2.43009600	-0.66132600	0.00000000
N -1.08369600	1.91969700	0.00000000	O 3.55948000	-1.02142300	0.00000000
H 0.97747800	0.60795000	0.00000000	Cr 0.84824900	-0.18526700	0.00000000
H -0.09224400	2.27825700	0.00000000	P 0.67674000	0.16151900	-2.32980400
C 1.93963000	1.41914600	0.00000000	P 0.67674000	0.16151900	2.32980400
C 3.16079700	0.58017000	0.00000000	C 0.92572200	2.00744700	-2.43974600
C 3.09346000	-0.81071800	0.00000000	C 0.92572200	2.00744700	2.43974600
C 4.24936000	-1.58244200	0.00000000	H -0.07327900	2.45265600	-2.41858700
C 5.49547500	-0.97089400	0.00000000	H -0.07327900	2.45265600	2.41858700
C 5.57495900	0.42013100	0.00000000	H 1.40946600	2.32250300	-3.36592200
C 4.42231100	1.18730600	0.00000000	H 1.40946600	2.32250300	3.36592200
P -0.67687700	0.15219000	2.33283100	C 1.70223200	2.47565700	-1.22110100
P -0.67687700	0.15219000	-2.33283100	C 1.70223200	2.47565700	1.22110100
N -0.34294700	-1.80998700	0.00000000	H 1.71173200	3.57443900	-1.18046300
C -2.55096500	-0.55356200	0.00000000	H 1.71173200	3.57443900	1.18046300
C 0.95867000	-0.06485600	-3.23321000	H 2.74092400	2.14002100	-1.25921500
C 0.95867000	-0.06485600	3.23321000	H 2.74092400	2.14002100	1.25921500
C -1.93967900	-0.62029400	-3.49936200	N 1.08304600	1.92764100	0.00000000
C -1.93967900	-0.62029400	3.49936200	C -0.94818000	-0.04917400	3.25204400
O -3.68138800	-0.82019400	0.00000000	C -0.94818000	-0.04917400	-3.25204400
C -0.92601900	1.99545500	2.43768500	H -1.65168200	0.44569500	2.57436600
C -0.92601900	1.99545500	-2.43768500	H -1.65168200	0.44569500	-2.57436600
H 0.07435500	2.43714500	2.41063300	C 1.96920500	-0.59475800	3.47019500
H 0.07435500	2.43714500	-2.41063300	C 1.96920500	-0.59475800	-3.47019500
H -1.40440600	2.31400600	3.36520000	C 3.32560800	0.10204700	3.37628300
H -1.40440600	2.31400600	-3.36520000	C 3.32560800	0.10204700	-3.37628300
C -1.70494300	2.46535700	1.22149800	C 0.23287200	-1.91444200	0.00000000
C -1.70494300	2.46535700	-1.22149800	O -0.09497200	-3.02486700	0.00000000
H -1.71178700	3.56400700	1.18037100	H 1.58289100	-0.45708500	-4.48610000
H -1.71178700	3.56400700	-1.18037100	H 1.58289100	-0.45708500	4.48610000
H -2.74459800	2.13280200	1.26110700	C 2.12548500	-2.09211200	-3.20148200
H -2.74459800	2.13280200	-1.26110700	C 2.12548500	-2.09211200	3.20148200
H 1.65590500	0.42407300	-2.54514600	H 1.18016300	-2.63237200	-3.24999300
H 1.65590500	0.42407300	2.54514600	H 1.18016300	-2.63237200	3.24999300
C -3.28859700	0.09586000	-3.49084200	H 2.55887000	-2.26701500	-2.21612200
C -3.28859700	0.09586000	3.49084200	H 2.55887000	-2.26701500	2.21612200
O -0.05754200	-2.95420000	0.00000000	H 2.79814900	-2.53024000	-3.94530300
H -1.50963500	-0.52568600	4.50232500	H 2.79814900	-2.53024000	3.94530300
H -1.50963500	-0.52568600	-4.50232500	C -1.37074000	-1.51036800	3.38464500
C -2.12485800	-2.10510300	3.18373500	C -1.37074000	-1.51036800	-3.38464500
C -2.12485800	-2.10510300	-3.18373500	H -0.77220900	-2.03247200	4.13537100
H -1.18522500	-2.65736400	3.18011500	H -0.77220900	-2.03247200	-4.13537100
H -1.18522500	-2.65736400	-3.18011500	H -1.28921900	-2.05386300	2.44309700
H -2.58985000	-2.24031300	2.20637800	H -1.28921900	-2.05386300	-2.44309700
H -2.58985000	-2.24031300	-2.20637800	H -2.41400600	-1.56267500	3.70768500
H -2.77905200	-2.56292600	3.93207000	H -2.41400600	-1.56267500	-3.70768500
H -2.77905200	-2.56292600	-3.93207000	C -1.00380900	0.65657500	4.60541100
C 1.36571700	-1.53188100	-3.35221700	C -1.00380900	0.65657500	-4.60541100
C 1.36571700	-1.53188100	3.35221700	H -0.77090600	1.72052400	4.53732400
H 0.77186100	-2.05070100	-4.10917500	H -0.77090600	1.72052400	-4.53732400
H 0.77186100	-2.05070100	4.10917500	H -0.32063400	0.20466400	5.32955500
H 1.26211100	-2.06857700	-2.40846700	H -0.32063400	0.20466400	-5.32955500
H 1.26211100	-2.06857700	2.40846700	H -2.01261500	0.57074600	5.02020500
H 2.41305400	-1.59957800	-3.65874700	H -2.01261500	0.57074600	-5.02020500
H 2.41305400	-1.59957800	3.65874700	H -0.99594600	0.55198300	0.00000000
C 1.04254000	0.63716400	-4.58669800	H 0.08872800	2.26778900	0.00000000
C 1.04254000	0.63716400	4.58669800	C -1.96275700	1.38560400	0.00000000
H 0.82003800	1.70385100	-4.52342400	C -3.19361900	0.55967600	0.00000000

H 0.82003800	1.70385100	4.52342400	C -3.15160600	-0.83145600	0.00000000
H 0.36584300	0.19189600	-5.32109000	C -4.31993200	-1.58433800	0.00000000
H 0.36584300	0.19189600	5.32109000	C -5.55561600	-0.95250600	0.00000000
H 2.05660500	0.54022200	-4.98610700	C -4.44576300	1.18704600	0.00000000
H 2.05660500	0.54022200	4.98610700	C -5.61113500	0.43964700	0.00000000
H 2.11759700	-1.28325500	0.00000000	H -2.18607000	-1.32221900	0.00000000
H 4.17310300	-2.66451300	0.00000000	H -4.26100200	-2.66748900	0.00000000
H 6.39953400	-1.57011100	0.00000000	H -6.46958300	-1.53643300	0.00000000
H 4.46669400	2.27096900	0.00000000	H -4.47233900	2.27122500	0.00000000
H 6.54454500	0.90718400	0.00000000	H -6.57211300	0.94342900	0.00000000
H -3.96613500	-0.39897900	4.19320800	H 4.02545900	-0.37487300	4.06912900
H -3.96613500	-0.39897900	-4.19320800	H 3.75151300	0.01409300	2.37533200
H -3.21421900	1.14099200	3.79680800	H 3.27706400	1.15906300	3.64440800
H -3.21421900	1.14099200	-3.79680800	H 4.02545900	-0.37487300	-4.06912900
H -3.75888900	0.05450300	2.50688500	H 3.27706400	1.15906300	-3.64440800
H -3.75888900	0.05450300	-2.50688500	H 3.75151300	0.01409300	-2.37533200
C 1.78417300	2.68424600	0.00000000	C -1.79852700	2.64726400	0.00000000
H 1.40732200	3.68138900	0.00000000	H -1.43308000	3.64832100	0.00000000
2Cr-cis + PhCHCH₂-TS-H_M transfer			2Cr-trans + PhCHCH₂-TS-H_M transfer		
O -2.37064800	2.24582500	-1.85906200	O -2.46130500	2.46536100	-1.36169900
P 1.04390600	1.94370400	-0.00269700	P 1.10927200	1.92077400	-0.02407200
P -2.34995000	-1.22982200	-0.05028800	P -2.36936700	-1.18432700	-0.06615500
C 2.09873400	1.01547200	-1.22956800	C 2.12546700	0.97874100	-1.27521600
C -1.53432500	-2.28944800	-1.35504700	C -1.59867800	-2.23731300	-1.40620500
H 2.74919000	0.34886500	-0.65686200	H 2.77125100	0.29331600	-0.71913700
H -0.94303500	-3.04156800	-0.82557800	H -1.02480300	-3.02222500	-0.90578500
H 2.74527200	1.67212500	-1.81471900	H 2.77479300	1.62637900	-1.86794300
H -2.25271600	-2.82484600	-1.97828200	H -2.34059400	-2.73149700	-2.03635400
C 1.20592800	0.19062000	-2.14039000	C 1.19786400	0.18158100	-2.17437600
C -0.61484600	-1.42962600	-2.20550600	C -0.66485400	-1.37970900	-2.24173300
H 1.81623500	-0.48431500	-2.75521000	H 1.78131600	-0.50402200	-2.80344300
H 0.00928900	-2.06457100	-2.84966500	H -0.06407700	-2.01345500	-2.90891400
H 0.63972100	0.83475200	-2.81749600	H 0.63644000	0.84372700	-2.83737600
H -1.19299400	-0.76929000	-2.85590200	H -1.23192100	-0.68723500	-2.86772700
N 0.23229400	-0.58283700	-1.34624600	N 0.21285500	-0.57200100	-1.37362300
C -2.49813000	-2.47533300	1.35734800	C -2.57594700	-2.48192000	1.28683700
C 2.20429500	2.03844800	1.47591500	C 2.33132400	2.02977800	1.40518100
H -1.45911300	-2.80723600	1.44857500	H -1.54506600	-2.83328900	1.40017700
H 2.39726400	0.97513200	1.64392300	H 2.46149700	0.96996100	1.64359100
C -4.12768200	-1.00472900	-0.63652100	C -4.12029000	-0.85809800	-0.67277400
C 0.98464700	3.71561300	-0.64413800	C 1.02738100	3.67594700	-0.69949400
C -4.24101500	-0.71818300	-2.13245600	C -4.16729400	-0.44201300	-2.14217900
C 0.78569800	3.80372800	-2.15603800	C 0.70784600	3.71731100	-2.19294700
O -2.12305100	1.87194400	2.33412000	O -1.78308200	1.62747400	2.73333500
H 1.96195100	4.14877200	-0.40864800	H 2.02931300	4.09433300	-0.55565600
H -4.62883500	-1.95730600	-0.43919600	H -4.65118100	-1.81053600	-0.57449800
C -0.09602800	4.51459600	0.08465800	C 0.02216600	4.52231100	0.08278400
C -4.81868500	0.09179700	0.17388700	C -4.81326900	0.18639300	0.20240600
H 0.02968700	4.50380800	1.16770600	H 0.21957400	4.52972100	1.15470200
H -4.79277500	-0.09816600	1.24754000	H -4.82828700	-0.09080100	1.25698300
H -1.08878200	4.11934400	-0.13545800	H -0.99490800	4.15935900	-0.06770700
H -4.34788600	1.06064400	0.00006600	H -4.31967900	1.15531900	0.11863400
H -0.07056600	5.55845900	-0.24283300	H 0.06276700	5.55799300	-0.26874500
H -5.86846400	0.16952000	-0.12492500	H -5.85096700	0.30944900	-0.12244500
C -2.89220300	-1.82609700	2.68130800	C -3.01565800	-1.90139700	2.62820600
C 1.53077800	2.58556700	2.73148600	C 1.76920200	2.71640000	2.64746600
H -3.94364600	-1.53017900	2.68828400	H -4.06578700	-1.60193600	2.61219000
H 1.36610000	3.66331900	2.66444800	H 1.71038700	3.79882500	2.51428200
H -2.29255400	-0.93974800	2.89224700	H -2.42411500	-1.03227000	2.91552900
H 0.56975500	2.10616400	2.91930200	H 0.77699100	2.35148000	2.91171000
H -2.75332300	-2.53636500	3.50215100	H -2.91026400	-2.65784600	3.41181500
H 2.17212200	2.41383300	3.60145300	H 2.43211500	2.53591400	3.49916100

C -3.35226500	-3.70512500	1.05833100	C -3.43509600	-3.68324400	0.89723800
C 3.54187100	2.72510100	1.21213500	C 3.69779700	2.60188100	1.03394700
H -3.09477800	-4.17587000	0.10653300	H -3.14168200	-4.12086500	-0.05940500
H 4.04546700	2.33792200	0.32375100	H 4.14783300	2.09766100	0.17698600
H -4.41786300	-3.46462200	1.03971200	H -4.49406200	-3.42080500	0.83909000
H 3.42771800	3.80553300	1.09526800	H 3.64218400	3.67014100	0.81041000
H -3.20884500	-4.45441900	1.84298700	H -3.34153600	-4.46531000	1.65688100
H 4.21206900	2.56725600	2.06292300	H 4.38556800	2.48916500	1.87777800
H 0.15517700	-0.44057000	1.13918700	H 0.13454400	-0.42890200	1.18810100
H 0.76331900	-1.21068600	-0.72507600	H 0.73230400	-1.22444600	-0.76742800
C 1.01924200	-1.60487000	1.77093100	C 0.92998200	-1.58419300	1.78426100
H -5.29734000	-0.62066400	-2.40114400	H -5.20927700	-0.28780900	-2.43871400
H -3.75070000	0.21663100	-2.40469300	H -3.63908600	0.49647800	-2.31242900
H -3.82710400	-1.51956300	-2.74773200	H -3.75414300	-1.20264800	-2.80767200
H 0.78142400	4.85527600	-2.45901700	H 0.68692300	4.75851400	-2.52893800
H 1.58409800	3.31189900	-2.71499500	H 1.45540300	3.19942100	-2.79696300
H -0.16895600	3.37574300	-2.46387000	H -0.27289300	3.28898500	-2.40450100
H 0.15986700	-1.91957600	2.34752000	H 0.07288000	-1.88326500	2.37485300
C 1.59216100	-2.50021500	0.88891200	C 1.47350300	-2.50794000	0.90548100
H 0.99143500	-3.34659300	0.56358300	H 0.84188500	-3.33294500	0.58407700
N -1.60593800	1.34885400	1.41352700	C -1.42356500	1.24212800	1.70164800
C -1.76920800	1.57268500	-1.12665600	N -1.77502000	1.66645500	-0.81208200
H 1.64692900	-0.89994300	2.30494500	H 1.59140200	-0.91533600	2.32612300
C 2.94027300	-2.46981800	0.35952200	C 2.81872500	-2.52749500	0.37503200
C 3.31554300	-3.38129700	-0.64778300	C 3.16393700	-3.46440000	-0.62115000
C 3.94162200	-1.59146000	0.81796600	C 3.84978700	-1.67544100	0.81942100
C 4.59694300	-3.40420800	-1.17214800	C 4.44306700	-3.53630700	-1.14561500
H 2.57566100	-4.08691100	-1.01443800	H 2.40125500	-4.15070000	-0.97770000
C 5.22239900	-1.61357700	0.28890400	C 5.12868100	-1.74772100	0.29040500
H 3.72123800	-0.90075900	1.62406000	H 3.65376200	-0.96683500	1.61614200
C 5.56411700	-2.51442800	-0.71480300	C 5.44005300	-2.67288600	-0.70099800
H 4.84529800	-4.12397400	-1.94537200	H 4.66663000	-4.27429300	-1.90921400
H 5.96876100	-0.92649200	0.67450300	H 5.89760000	-1.08037700	0.66633400
H 6.56802600	-2.53145500	-1.12285500	H 6.44243700	-2.72864200	-1.10924800
Cr -0.87276000	0.59445400	0.12854800	Cr -0.84941000	0.61988400	0.08528800
2Cr-cis + PhCHCH₂-interm			2Cr-trans + PhCHCH₂-interm		
O -2.36227900	2.23734100	-1.80512600	O -2.44196300	2.39478200	-1.44148500
P 1.06820300	1.92865000	-0.01570200	P 1.10342300	1.91564200	-0.02269700
P -2.40557400	-1.22656300	-0.03532700	P -2.39833600	-1.20987100	-0.05008600
C 2.10778200	0.95161400	-1.20845200	C 2.12534600	0.93969000	-1.23616600
C -1.58745500	-2.30522600	-1.31524000	C -1.61377900	-2.27095700	-1.37062000
H 2.74163700	0.28701100	-0.61461500	H 2.75768100	0.26085100	-0.65663400
H -1.01988300	-3.06133600	-0.76719300	H -1.05184500	-3.05461400	-0.85630100
H 2.77036400	1.57825000	-1.80806600	H 2.78819100	1.56866800	-1.83372600
H -2.30218700	-2.83222500	-1.94950800	H -2.34887600	-2.76418400	-2.00927200
C 1.20126900	0.11686100	-2.09476300	C 1.20301900	0.12737700	-2.12668800
C -0.63270700	-1.46821600	-2.14891400	C -0.66007800	-1.42396500	-2.19507100
H 1.80295300	-0.59635700	-2.67236600	H 1.79197600	-0.58227500	-2.72183900
H 0.00741600	-2.12469900	-2.75353300	H -0.04049000	-2.07042700	-2.83119900
H 0.65935300	0.74552600	-2.80569000	H 0.66048300	0.77326900	-2.82106900
H -1.18082400	-0.82092500	-2.83761800	H -1.21060900	-0.74690300	-2.85220000
N 0.20534500	-0.61462100	-1.28003200	N 0.20077600	-0.60170900	-1.31893100
C -2.59739500	-2.44679700	1.38690800	C -2.60665100	-2.48293700	1.32466400
C 2.20974200	2.06636100	1.47265900	C 2.29156200	2.06306200	1.42991600
H -1.55739800	-2.74801000	1.54702300	H -1.57646300	-2.83350700	1.44576200
H 2.31042500	1.01540400	1.75863800	H 2.38161900	1.01704300	1.73756500
C -4.16887700	-0.94662400	-0.63586100	C -4.14467500	-0.87871000	-0.66389200
C 0.99716400	3.68313500	-0.69781700	C 1.01249400	3.65580500	-0.73259800
C -4.26650000	-0.70576400	-2.14111000	C -4.18940900	-0.49426000	-2.14204500
C 0.84413100	3.73439500	-2.21681400	C 0.74662300	3.66709800	-2.23710800
O -2.05896400	1.85879700	2.37667300	O -1.86755300	1.71263100	2.67711900
H 1.96394500	4.12880100	-0.44152900	H 2.00408500	4.08815100	-0.56045200

H -4.70208200	-1.87522800	-0.40956700	H -4.67945700	-1.82660700	-0.54586400
C -0.10900200	4.49294000	-0.02017100	C -0.02763500	4.50579700	-0.00128000
C -4.82755700	0.19615800	0.13734700	C -4.83364900	0.18506800	0.19083000
H -0.03636100	4.48184600	1.06729100	H 0.11953800	4.51947300	1.07835000
H -4.79114900	0.05131100	1.21745600	H -4.84589800	-0.06923500	1.25114200
H -1.09475100	4.11250400	-0.28952500	H -1.03728900	4.14434100	-0.19699300
H -4.34478000	1.14886900	-0.08390900	H -4.34102900	1.15232700	0.08502500
H -0.05410000	5.53582500	-0.34689300	H 0.03045200	5.53917800	-0.35678200
H -5.87945100	0.27935600	-0.15198000	H -5.87208900	0.30151300	-0.13360600
C -3.09198100	-1.79135000	2.67380000	C -3.04860300	-1.88159500	2.65587600
C 1.57701900	2.80683700	2.64863900	C 1.72385700	2.84619400	2.61136100
H -4.15194100	-1.53438400	2.61266100	H -4.09593100	-1.57306500	2.63177200
H 1.53182700	3.88311800	2.46710800	H 1.71205400	3.91975600	2.41056900
H -2.53703800	-0.88320000	2.91203800	H -2.44929600	-1.01554600	2.93674200
H 0.56824400	2.45440300	2.86695900	H 0.71181300	2.53578600	2.87161300
H -2.97856400	-2.48615400	3.51121800	H -2.95276700	-2.62949700	3.44857600
H 2.18558600	2.65973900	3.54576200	H 2.35716900	2.69290700	3.49009100
C -3.40110000	-3.70217600	1.05502400	C -3.46626400	-3.68806100	0.94809500
C 3.60275800	2.60704400	1.15930000	C 3.68388500	2.56708800	1.05592000
H -3.06265800	-4.18999100	0.13838500	H -3.16993000	-4.13847000	-0.00159200
H 4.09675400	2.05456900	0.35824400	H 4.14535100	1.97796800	0.26205300
H -4.46726700	-3.48686600	0.95130300	H -4.52497000	-3.42585800	0.88413900
H 3.57674000	3.66390200	0.88203100	H 3.66594100	3.61351000	0.74087400
H -3.30054100	-4.42835700	1.86731400	H -3.37441700	-4.45985000	1.71814000
H 4.23538900	2.52694000	2.04856600	H 4.34088400	2.50836100	1.92898800
H 0.31504800	-0.63162000	1.23838800	H 0.26578100	-0.60544500	1.23456800
H 0.76853100	-1.29328300	-0.67135600	H 0.73747000	-1.28018700	-0.71274100
C 0.96239600	-1.54007400	1.65160200	C 0.90849700	-1.53431300	1.67674000
H -5.31734200	-0.57521600	-2.41649400	H -5.23107900	-0.34599800	-2.44225300
H -3.73912500	0.19959800	-2.44284700	H -3.66062100	0.43975700	-2.33329900
H -3.88287500	-1.54274000	-2.72737700	H -3.77617100	-1.26918100	-2.79037800
H 0.83466200	4.77866500	-2.54326300	H 0.72464600	4.70207700	-2.59132200
H 1.66509500	3.24071100	-2.73955800	H 1.52124600	3.14843500	-2.80469900
H -0.09535300	3.28648700	-2.54366600	H -0.22051700	3.22265600	-2.47686300
H 0.24039700	-2.03999900	2.29755200	H 0.15976700	-1.98990800	2.32410800
C 1.55333300	-2.39142600	0.63408800	C 1.48870300	-2.42501900	0.70226100
H 0.98536300	-3.27057900	0.33964600	H 0.89044600	-3.27716600	0.38964800
N -1.56365000	1.32633200	1.45103300	C 2.86279000	-2.46394800	0.30524900
C 2.93998900	-2.41956500	0.27470800	C 3.30160400	-3.42763600	-0.63907900
C 3.41078800	-3.37503000	-0.66228800	C 3.86442500	-1.59588800	0.80389600
C 3.92071200	-1.54264200	0.79788700	C 4.61610400	-3.50529100	-1.05473200
C 4.73432800	-3.43510400	-1.05094800	H 2.57383400	-4.12845500	-1.03883100
H 2.70008000	-4.08307400	-1.07971600	C 5.18215100	-1.67948100	0.38062500
C 5.24831800	-1.60834200	0.40176900	H 3.61178700	-0.86537600	1.56460500
H 3.64392600	-0.81634700	1.55435900	C 5.57869900	-2.62596400	-0.55779900
C 5.67595900	-2.54589500	-0.53138100	H 4.90043300	-4.26409600	-1.77740500
H 5.04286000	-4.18830400	-1.76962000	H 5.91575000	-0.99833100	0.80150300
H 5.96435900	-0.91966700	0.84039800	H 6.61021700	-2.68824800	-0.88369500
H 6.71467400	-2.59438900	-0.83615400	H 1.62615400	-1.00645000	2.30618300
H 1.68227800	-1.02837100	2.29228700	Cr -0.86581000	0.60169500	0.08603400
Cr -0.86663600	0.56993000	0.14092200	C -1.47086500	1.27324900	1.68323500
C -1.76550300	1.56518300	-1.06975100	N -1.77715700	1.62768800	-0.82973800
2Cr-cis + PhCHCH₂-TS-H_N transfer			2Cr-trans + PhCHCH₂-TS-H_N transfer		
O -2.34845000	2.16042600	-1.87973700	O -2.46895200	2.30486300	-1.51805400
P 1.04771800	1.93728000	-0.02000800	P 1.06190700	1.93342100	-0.03144800
P -2.40785100	-1.24606700	-0.01918200	P -2.40426600	-1.24891800	-0.02888800
C 2.10485600	0.95190700	-1.18578900	C 2.11454900	0.94331000	-1.19927500
C -1.54958900	-2.35702100	-1.23879100	C -1.55386600	-2.35637200	-1.26007000
H 2.74882400	0.31531500	-0.57337900	H 2.76334900	0.30779400	-0.59085000
H -0.99181800	-3.08832000	-0.64965100	H -1.00503300	-3.10467700	-0.68414000
H 2.75707200	1.57426000	-1.80090500	H 2.76079200	1.56762400	-1.81940300
H -2.24247600	-2.91155500	-1.87384000	H -2.25558000	-2.89092700	-1.90319300

C	1.21146100	0.07507800	-2.04518700	C	1.21427600	0.06675300	-2.05071800
C	-0.57857100	-1.53505100	-2.07006000	C	-0.57674100	-1.52996100	-2.07907800
H	1.82815300	-0.66402400	-2.57371600	H	1.82709800	-0.67725300	-2.57762400
H	0.10142700	-2.20875100	-2.61019100	H	0.10406700	-2.20202800	-2.62091700
H	0.69209000	0.66853300	-2.80382800	H	0.69760500	0.66029800	-2.81164900
H	-1.11291300	-0.94703300	-2.82216300	H	-1.10773500	-0.93759600	-2.83073000
N	0.20687000	-0.62240200	-1.21447100	N	0.20428400	-0.61903800	-1.21893900
C	-2.62367400	-2.40732400	1.44736400	C	-2.64636600	-2.44437900	1.40785400
C	2.16779700	2.10272300	1.48206600	C	2.21711600	2.13038100	1.44199700
H	-1.58291100	-2.66636500	1.66619000	H	-1.61167300	-2.73925300	1.61193000
H	2.27111900	1.05650100	1.78535500	H	2.32192900	1.09115500	1.76927900
C	-4.15876000	-0.99525800	-0.66575000	C	-4.12982700	-0.96764100	-0.71981200
C	0.96184800	3.68281400	-0.72110100	C	0.94867400	3.65283800	-0.78370000
C	-4.22390900	-0.81518000	-2.18128500	C	-4.12032900	-0.65323500	-2.21525800
C	0.83118000	3.71473300	-2.24282300	C	0.69659400	3.61836300	-2.29046600
O	-2.10739600	1.89181400	2.32415400	O	-1.94914200	1.75191800	2.62622300
H	1.91863500	4.14430000	-0.45527500	H	1.93263600	4.10368900	-0.61491400
H	-4.69368900	-1.91635900	-0.41333800	H	-4.65648200	-1.91713000	-0.57810000
C	-0.16479200	4.48492800	-0.06859600	C	-0.10912200	4.50717000	-0.08377500
C	-4.83826700	0.17469600	0.04655400	C	-4.86653400	0.12381400	0.05670800
H	-0.10871200	4.48572600	1.01993000	H	0.02968200	4.55267400	0.99612400
H	-4.81544000	0.07901400	1.13237500	H	-4.91320500	-0.07890200	1.12689800
H	-1.14143100	4.08901200	-0.34872800	H	-1.11224100	4.12640700	-0.27658300
H	-4.36157000	1.12123800	-0.21092800	H	-4.38743800	1.09395100	-0.07885000
H	-0.11848200	5.52502000	-0.40538200	H	-0.06341600	5.53108500	-0.46724900
H	-5.88666200	0.23466900	-0.26074700	H	-5.89417400	0.20528600	-0.31007000
C	-3.19690300	-1.71597800	2.68202200	C	-3.19704900	-1.79252900	2.67336100
C	1.51701000	2.85759200	2.63888700	C	1.61662100	2.92261100	2.60092100
H	-4.26101500	-1.49922500	2.56336300	H	-4.25510600	-1.54226900	2.57037100
H	1.46742700	3.93058900	2.43959000	H	1.58792300	3.99225000	2.38162700
H	-2.68320900	-0.78076500	2.90720000	H	-2.65881800	-0.88314300	2.93949100
H	0.50783900	2.50286600	2.85150000	H	0.60674800	2.59827600	2.85203700
H	-3.09904300	-2.37201000	3.55204600	H	-3.11339700	-2.48978700	3.51225800
H	2.11600000	2.72872000	3.54522800	H	2.23916800	2.79643000	3.49158800
C	-3.37423900	-3.70025300	1.13538500	C	-3.43197400	-3.70483500	1.05091700
C	3.56106800	2.64777500	1.17700000	C	3.60544900	2.65530300	1.08144200
H	-2.97324500	-4.22109000	0.26343500	H	-3.05315600	-4.19939600	0.15431700
H	4.06752100	2.08732000	0.38941500	H	4.08878900	2.06548100	0.30126500
H	-4.43844500	-3.52104100	0.96405000	H	-4.49234900	-3.48996200	0.89823600
H	3.53096300	3.70023400	0.88375900	H	3.57185100	3.69719700	0.75287400
H	-3.29947700	-4.38342800	1.98686500	H	-3.36707900	-4.42378800	1.87311300
H	4.18404500	2.58523700	2.07448400	H	4.25095600	2.62007900	1.96429800
H	0.33261400	-0.65368200	1.35175000	H	0.31048400	-0.65621500	1.36770000
H	0.84979500	-1.35135200	-0.54933700	H	0.85269100	-1.36358200	-0.53467000
C	1.00647900	-1.54188500	1.65819100	C	0.98896900	-1.54456300	1.66576200
H	-5.26837400	-0.69589400	-2.48464400	H	-5.15062200	-0.53050500	-2.56255300
H	-3.68910700	0.07742500	-2.50744800	H	-3.59254500	0.27640600	-2.42993500
H	-3.82720600	-1.67452200	-2.72463600	H	-3.67347100	-1.45250000	-2.80909000
H	0.81180900	4.75507300	-2.58120900	H	0.66275000	4.64272400	-2.67347700
H	1.66664000	3.22652600	-2.74713700	H	1.48364400	3.09496000	-2.83578000
H	-0.09624000	3.24904400	-2.57888400	H	-0.26078700	3.15195300	-2.52704200
H	0.35373500	-2.13420800	2.30179600	H	0.33888500	-2.13982200	2.30956300
C	1.56116300	-2.28336800	0.50903600	C	1.53522700	-2.27688300	0.50633500
H	1.04635400	-3.21628100	0.28185500	H	1.01882600	-3.21019200	0.28260600
N	-1.59497200	1.33821400	1.42035000	Cr	-0.89128700	0.58261000	0.07676300
C	-1.76759800	1.52451100	-1.10187100	C	-1.52512500	1.28287000	1.65848400
H	1.75662100	-1.07772500	2.30087400	N	-1.81234300	1.58339000	-0.84818100
C	2.98251700	-2.35425900	0.22803300	H	1.74194300	-1.08192200	2.30616400
C	3.46562500	-3.30044000	-0.70527400	C	2.96012000	-2.36177800	0.23166700
C	3.95509600	-1.51358200	0.80859600	C	3.43609700	-3.30880400	-0.70313900
C	4.80323600	-3.38630800	-1.04191500	C	3.93761800	-1.53283900	0.81846700
H	2.75594700	-3.98218500	-1.16598000	C	4.77434300	-3.40775200	-1.03477100
C	5.29841800	-1.60141400	0.46716100	H	2.72113700	-3.98131400	-1.16915700

H 3.66304600	-0.79034700	1.56231400	C 5.28164500	-1.63304900	0.48234700
C 5.74124700	-2.53108300	-0.46462500	H 3.64960700	-0.80902400	1.57317400
H 5.12400300	-4.13305800	-1.76176400	C 5.71833500	-2.56445800	-0.45036000
H 6.01057900	-0.93724300	0.94752000	H 5.09034900	-4.15516500	-1.75597300
H 6.79059500	-2.59911300	-0.72682300	H 5.99859700	-0.97762800	0.96747000
Cr -0.87717100	0.55925200	0.13196000	H 6.76806100	-2.64266900	-0.70826100
2Cr-cis + PhCHO-TS-H_M transfer			2Cr-trans + PhCHO -TS-H_M transfer		
O 2.24797100	3.01572800	-0.14860800	O 2.05568800	2.95486700	-0.69221600
Cr 0.63610900	0.50019800	-0.23398500	Cr 0.62480200	0.54577700	-0.20180400
P -1.37162500	1.67581700	0.10941600	P -1.43818900	1.63616800	0.13693400
P 2.53757600	-0.87254800	0.10476800	P 2.56980000	-0.79316200	0.12383600
C -1.62727300	1.43074600	1.93896200	C -1.66275400	1.40892900	1.97514000
C 2.61036600	-1.01885500	1.96375700	C 2.68203900	-0.87600100	1.98580800
H -2.17415100	0.48963400	2.04874700	H -2.19360800	0.46132000	2.10742500
H 2.08948200	-1.94495000	2.22060600	H 2.21692200	-1.81914900	2.28352500
H -2.23120200	2.21714000	2.39625300	H -2.27181600	2.19295400	2.43065000
H 3.62983100	-1.08915900	2.34631100	H 3.71093700	-0.87540600	2.35005700
C -0.27642200	1.31311900	2.62492900	C -0.30032600	1.32636300	2.64078600
C 1.87021700	0.15193300	2.58930800	C 1.89142500	0.27681500	2.57948100
H -0.41119900	1.04346800	3.68176600	H -0.41329300	1.05333800	3.69947100
H 1.74795400	-0.01650600	3.66843900	H 1.79384200	0.14298900	3.66613400
H 0.25638200	2.26683600	2.59717600	H 0.20396100	2.29479000	2.60696800
H 2.42625300	1.08429000	2.46240200	H 2.39703400	1.23032600	2.40807400
N 0.55415100	0.30672000	1.94517800	N 0.55926400	0.35045500	1.95161400
C 2.52867900	-2.69137100	-0.38676100	C 2.66105000	-2.62847300	-0.29302900
C -2.97245600	0.99730400	-0.59650800	C -3.06310000	0.95298500	-0.51447600
H 1.68116100	-3.06039000	0.19859300	H 1.83466300	-3.01932100	0.30897800
H -2.90293700	-0.05270700	-0.30131100	H -2.97778300	-0.10142300	-0.23829300
C 4.24936900	-0.28447400	-0.42733300	C 4.23272900	-0.10794100	-0.43055900
C -1.52321000	3.53581400	-0.17274400	C -1.58384500	3.49410300	-0.13807300
C 4.85073500	0.77363900	0.49554200	C 4.70496400	1.07508200	0.41343700
C -0.86750200	4.37943000	0.91863200	C -0.80516800	4.31473700	0.88835100
O 0.61384300	0.44214000	-3.06971900	O 0.27323200	-0.02368200	-3.10955600
H -2.59804200	3.74417200	-0.15659900	H -2.64813600	3.72256800	-0.01547700
H 4.89085300	-1.16948200	-0.37979900	H 4.94723200	-0.92510900	-0.28985000
C -0.97300800	3.92293900	-1.54637100	C -1.16013000	3.88019000	-1.55645400
C 4.21575500	0.21679000	-1.87099700	C 4.20050600	0.26630500	-1.91222400
H -1.41593900	3.34471300	-2.35724300	H -1.69061000	3.31710500	-2.32372600
H 3.81686000	-0.52417600	-2.56497600	H 3.89589000	-0.56507900	-2.54910700
H 0.10686200	3.77850300	-1.59028000	H -0.09166200	3.72199500	-1.70312900
H 3.59975600	1.11290600	-1.95908900	H 3.51166000	1.09264300	-2.09135000
H -1.17618700	4.98058600	-1.74140600	H -1.36578300	4.94232200	-1.72307200
H 5.22792200	0.47102500	-2.20035300	H 5.19671800	0.58384500	-2.23527700
C 2.20577600	-2.89640700	-1.86429100	C 2.36764200	-2.93220300	-1.75955100
C -3.01064000	1.04267900	-2.12212800	C -3.18692600	1.02097000	-2.03501300
H 3.04587000	-2.61396700	-2.50313300	H 3.19721800	-2.63724300	-2.40611200
H -3.16783400	2.05880600	-2.49232100	H -3.39628600	2.03742000	-2.37660100
H 1.33814400	-2.31089100	-2.17243300	H 1.47163800	-2.42076900	-2.11269400
H -2.09455600	0.65286500	-2.56753900	H -2.28931600	0.66670400	-2.54199000
H 1.99436400	-3.95222500	-2.05989200	H 2.22149200	-4.00814800	-1.89547800
H -3.84492300	0.43555000	-2.48492800	H -4.02246100	0.39435600	-2.35942200
C 3.75741900	-3.49267900	0.03715000	C 3.93580200	-3.32903300	0.17333000
C -4.24632600	1.58424700	0.00622400	C -4.31003400	1.52417300	0.15751100
H 4.01239800	-3.34418900	1.08889600	H 4.17019100	-3.12273600	1.21977500
H -4.26100200	1.52738700	1.09650000	H -4.28260100	1.43439700	1.24488100
H 4.63497500	-3.24325300	-0.56416300	H 4.80034900	-3.04562900	-0.43176600
H -4.39385600	2.62860100	-0.28140900	H -4.46414900	2.57709200	-0.09299800
H 3.56743900	-4.56108100	-0.10498600	H 3.81711700	-4.41227100	0.07317700
H -5.11317600	1.02620100	-0.35973000	H -5.19248100	0.97955900	-0.19093700
H -0.43718100	-0.87365800	-0.11604600	H -0.41326300	-0.89128500	-0.16433200
H 0.07754100	-0.60551400	2.03491900	H 0.13149400	-0.58574300	2.05385100
C -0.91114600	-2.39441200	0.72643600	C -0.75924900	-2.37764600	0.63240200

C	-2.34099000	-2.46961300	0.31038200	C	-2.20399800	-2.50004100	0.27066800
C	-2.67379200	-2.74347400	-1.01574900	C	-2.58242000	-2.75242900	-1.04737300
C	-4.00057400	-2.89877500	-1.38782500	C	-3.91721200	-2.94950300	-1.36827800
C	-5.00721900	-2.78882000	-0.43302300	C	-4.88618900	-2.90246200	-0.37040400
C	-3.35213400	-2.37298600	1.26497800	C	-3.17656300	-2.46797500	1.26823900
C	-4.68046000	-2.52821200	0.89345100	C	-4.51298000	-2.66424600	0.94795600
H	-1.88426700	-2.81965900	-1.75695400	H	-1.82373400	-2.78192200	-1.82344200
H	-4.25318100	-3.10866900	-2.42129900	H	-4.20479000	-3.14317900	-2.39577600
H	-6.04481100	-2.91530400	-0.72215500	H	-5.92960900	-3.06159700	-0.61966000
H	-3.07260300	-2.19813800	2.29781400	H	-2.85946100	-2.31071000	2.29299900
H	-5.46381600	-2.45798500	1.64034700	H	-5.26578100	-2.64420900	1.72859700
H	5.84820600	1.04145100	0.13347600	H	5.68864000	1.39835700	0.05904100
H	4.25654400	1.68739700	0.50943500	H	4.03274900	1.92892200	0.32735500
H	4.96649500	0.41968300	1.52168900	H	4.81241200	0.81980800	1.46937400
H	-1.01784400	5.44033400	0.69589800	H	-0.93628800	5.37992700	0.67447000
H	-1.29342500	4.19475300	1.90674700	H	-1.15130400	4.14664300	1.91009500
H	0.20945600	4.21117700	0.96629800	H	0.26470100	4.10507300	0.84046800
O	-0.57835800	-2.26446100	1.91526700	O	-0.38896600	-2.28753300	1.81785100
H	-0.23095600	-2.85705500	-0.00253400	H	-0.09778000	-2.82080400	-0.12724700
N	0.62571600	0.47678100	-1.89327900	C	0.41611900	0.21069700	-1.98551000
C	1.63746000	2.02742200	-0.14396800	N	1.48184600	1.94868100	-0.43411600
2Cr-cis + PhCHO-interm				2Cr-trans + PhCHO-interm			
O	2.14252500	3.02633400	-0.26363800	O	2.09458300	2.93349100	-0.56934300
Cr	0.60085700	0.48807600	-0.22285300	Cr	0.63312100	0.54177600	-0.19890900
P	-1.45448100	1.64134300	0.12572800	P	-1.45047000	1.65371200	0.13636100
P	2.57690200	-0.82290400	0.11875900	P	2.57735400	-0.83178800	0.13004000
C	-1.69983000	1.33820200	1.94216800	C	-1.70147300	1.34090600	1.95203600
C	2.64850900	-0.92989100	1.97424400	C	2.64290400	-0.94486300	1.98610000
H	-2.21309600	0.37541500	2.02099700	H	-2.22953900	0.38557300	2.02584900
H	2.16217600	-1.87270900	2.23585100	H	2.15893300	-1.88873600	2.24765300
H	-2.32937100	2.09173300	2.41999800	H	-2.32056100	2.10167100	2.43259900
H	3.66775000	-0.94546500	2.36273400	H	3.66226500	-0.95647000	2.37544400
C	-0.34573700	1.23918500	2.62382600	C	-0.34959900	1.22036700	2.63319800
C	1.84422500	0.21265600	2.57145600	C	1.83528900	0.19832900	2.57595700
H	-0.47828700	0.88689800	3.65607700	H	-0.48789800	0.85675900	3.66105800
H	1.69413100	0.03090800	3.64471100	H	1.68301600	0.02012300	3.64974400
H	0.13470700	2.22066900	2.67835900	H	0.13734700	2.19780600	2.70166400
H	2.37528200	1.16462100	2.47610100	H	2.36689800	1.15010200	2.47829100
N	0.53761300	0.31448200	1.89575900	N	0.53218200	0.30352100	1.89505000
C	2.61289700	-2.64439200	-0.34730000	C	2.63050400	-2.65530800	-0.32978800
C	-3.03764500	0.95118000	-0.60634500	C	-3.06045500	1.00902300	-0.58481700
H	1.73796500	-3.01557300	0.19472700	H	1.76333500	-3.03240400	0.22161400
H	-2.96015100	-0.10572700	-0.33716000	H	-2.99729900	-0.05698000	-0.34702600
C	4.25024500	-0.17465600	-0.45450400	C	4.24708800	-0.15081000	-0.40319100
C	-1.61635500	3.50239400	-0.11783000	C	-1.55347700	3.52007900	-0.07649800
C	4.83897700	0.90004800	0.45750100	C	4.73905100	0.99349300	0.48210300
C	-0.94849600	4.32415000	0.98269600	C	-0.79045000	4.29032300	0.99945900
O	0.53411200	0.35395100	-3.05806800	O	0.38061400	0.11751100	-3.15521300
H	-2.69318500	3.69602600	-0.07273100	H	-2.61784700	3.75455200	0.03246000
H	4.91712400	-1.04162300	-0.42048300	H	4.94498200	-0.98629300	-0.28870300
C	-1.10406200	3.92942600	-1.49399800	C	-1.09878600	3.95544400	-1.47067000
C	4.17461500	0.32132600	-1.89859400	C	4.22787600	0.27110200	-1.87233400
H	-1.56080600	3.36694200	-2.30805900	H	-1.61359000	3.42227200	-2.26930400
H	3.76136900	-0.42374800	-2.57929500	H	3.89387000	-0.52760700	-2.53542800
H	-0.02375500	3.80344000	-1.56901200	H	-0.02749900	3.80305700	-1.60158300
H	3.55532700	1.21595100	-1.97517800	H	3.57111600	1.12809700	-2.02628000
H	-1.32619800	4.98860100	-1.65620700	H	-1.30002500	5.02309300	-1.60227900
H	5.17701300	0.57820600	-2.25430800	H	5.23506100	0.56253300	-2.18531800
C	2.38877800	-2.88229400	-1.83790800	C	2.40546000	-2.92046900	-1.81539700
C	-3.08331800	1.03511200	-2.13015600	C	-3.14961700	1.13750700	-2.10368400
H	3.26368300	-2.59777400	-2.42747700	H	3.27262700	-2.63134600	-2.41371200
H	-3.27939100	2.05397300	-2.47295900	H	-3.35231200	2.16649300	-2.40979000

H	1.53042000	-2.32577400	-2.21722300	H	1.53631300	-2.38756100	-2.20216400
H	-2.15827000	0.68996200	-2.59361500	H	-2.24174100	0.80323000	-2.60650000
H	2.20893800	-3.94560900	-2.02181100	H	2.24351100	-3.98983700	-1.97942900
H	-3.89727500	0.40743500	-2.50323100	H	-3.97678000	0.52339300	-2.46994200
C	3.83179100	-3.40949100	0.16412400	C	3.86405300	-3.39500500	0.18464000
C	-4.31864200	1.50260500	0.01581300	C	-4.31547100	1.56632500	0.08423800
H	4.00630300	-3.25508000	1.23081300	H	4.04311500	-3.22433900	1.24796100
H	-4.32965200	1.41285500	1.10352800	H	-4.31130300	1.42961600	1.16673600
H	4.74298500	-3.13707600	-0.37424800	H	4.76680000	-3.11457700	-0.36376100
H	-4.48335400	2.55198800	-0.24296300	H	-4.45502400	2.63003000	-0.12636500
H	3.67982400	-4.48224800	0.01123100	H	3.72728400	-4.47165300	0.04632000
H	-5.17597800	0.93970300	-0.36411600	H	-5.19387700	1.04349600	-0.30460500
H	-0.55267900	-1.05230900	-0.02924900	H	-0.57817200	-1.05965800	-0.07755600
H	0.09085700	-0.69826000	1.96477500	H	0.08862000	-0.71468300	1.94099000
C	-0.76449300	-2.10790900	0.54247200	C	-0.76484800	-2.10669800	0.48832400
C	-2.22000000	-2.40406200	0.22375400	C	-2.22773300	-2.41470500	0.19936300
C	-2.63668900	-2.63815600	-1.08641900	C	-2.67262400	-2.65056500	-1.10112300
C	-3.96020000	-2.95279300	-1.36141700	C	-4.00164600	-2.96625500	-1.34765400
C	-4.88441000	-3.04302600	-0.32435900	C	-4.90377700	-3.05619200	-0.29136700
C	-3.14499600	-2.50946700	1.25684400	C	-3.13078100	-2.52058700	1.25153100
C	-4.47165700	-2.82503200	0.98437900	C	-4.46311800	-2.83666900	1.00789000
H	-1.91659400	-2.57142400	-1.89750700	H	-1.97055100	-2.58575100	-1.92816700
H	-4.27269600	-3.13432100	-2.38437200	H	-4.33542100	-3.14938900	-2.36360100
H	-5.91785700	-3.29449000	-0.53681300	H	-5.94130000	-3.30870800	-0.48156100
H	-2.78812100	-2.36470200	2.27038800	H	-2.75276100	-2.37496300	2.25731900
H	-5.18421500	-2.91160300	1.79816600	H	-5.15812600	-2.92305000	1.83678300
H	5.81802400	1.20117400	0.07253000	H	5.72831800	1.31192100	0.13952900
H	4.21613200	1.79438500	0.48925900	H	4.08216700	1.86185600	0.42664300
H	4.98929200	0.54690400	1.47909100	H	4.83944200	0.69987600	1.52833500
H	-1.11667800	5.38826000	0.79097900	H	-0.90820800	5.36420300	0.82566400
H	-1.35320500	4.10639100	1.97267000	H	-1.16108400	4.08292200	2.00481200
H	0.13109000	4.16832200	1.00645400	H	0.27846400	4.07303500	0.96897800
O	-0.43485700	-2.05554500	1.81661900	O	-0.40893700	-2.06567500	1.76058700
H	-0.15232800	-2.77897600	-0.08839100	H	-0.16413000	-2.77726700	-0.15676800
N	0.56031600	0.41334700	-1.88545200	C	0.46851600	0.26942900	-2.01461100
C	1.55084600	2.02998500	-0.23099600	N	1.49381900	1.92880300	-0.40780700
2Cr-cis + PhCHO-TS-H_N transfer				2Cr-trans + PhCHO-TS-H_N transfer			
O	2.25073100	2.98661900	-0.14210200	N	1.56130500	1.90002100	-0.41433700
Cr	0.63598800	0.50171900	-0.22078200	O	2.19349900	2.88635500	-0.56678600
P	-1.40261300	1.69143100	0.11489900	Cr	0.66723900	0.53847500	-0.19316100
P	2.56287300	-0.88147000	0.11995800	P	-1.39511800	1.69910700	0.12812700
C	-1.71254500	1.30787300	1.90474700	P	2.56624700	-0.89039100	0.13190400
C	2.59534000	-1.04431000	1.97142500	C	-1.66601100	1.39353800	1.94047200
H	-2.25463900	0.35789700	1.92001400	C	2.58031800	-1.06869500	1.98232900
H	2.09942300	-1.99119900	2.19626400	H	-2.23172500	0.45999500	2.01101300
H	-2.33665200	2.05491200	2.39983500	H	2.05796200	-2.00222500	2.20465500
H	3.60656600	-1.07732300	2.37909500	H	-2.25469900	2.17852000	2.42024100
C	-0.38271700	1.13634500	2.61868700	H	3.58910000	-1.13065800	2.39438300
C	1.78542800	0.08807600	2.58077800	C	-0.32025900	1.21309700	2.62079700
H	-0.55851700	0.72220400	3.62160100	C	1.79879100	0.08584800	2.58653600
H	1.59401200	-0.13368900	3.64019100	H	-0.47853100	0.83507700	3.64126900
H	0.10962700	2.10504600	2.75670400	H	1.60177600	-0.12898500	3.64677300
H	2.34059000	1.03174200	2.54689300	H	0.19673200	2.17448500	2.71554500
N	0.50701300	0.24091500	1.86490700	H	2.38077700	1.01383200	2.55205100
C	2.53552700	-2.68870200	-0.39910200	N	0.52672700	0.27586000	1.87030200
C	-2.97525800	1.06713500	-0.69765300	C	2.57886800	-2.69731800	-0.39565900
H	1.64363900	-3.04124800	0.12777600	C	-3.01349100	1.08988100	-0.60654700
H	-2.93709900	0.00083900	-0.45575600	H	1.69258000	-3.07158300	0.12660700
C	4.26637200	-0.27669100	-0.40921300	H	-2.97882700	0.02374400	-0.36208000
C	-1.51162300	3.56456600	-0.04350700	C	4.26827200	-0.23904900	-0.32924000
C	4.87399300	0.75461000	0.53983800	C	-1.44712800	3.56656400	-0.08698400
C	-0.83857800	4.31210900	1.10580700	C	4.74628500	0.88207800	0.59266800

O	0.63730600	0.46058000	-3.06139600	C	-0.66236400	4.31288400	0.99034400
H	-2.58347600	3.78472100	-0.00347800	C	0.49458900	0.26621300	-2.01040200
H	4.90269600	-1.16663700	-0.38632200	O	0.40691800	0.12426500	-3.15253600
C	-0.96686400	4.04285800	-1.38998000	H	-2.50462200	3.83035100	0.02254200
C	4.23150200	0.25762300	-1.84113600	H	4.94338500	-1.09079100	-0.19828000
H	-1.43010200	3.53684200	-2.23680900	C	-0.98035600	3.99003900	-1.48065000
H	3.80629300	-0.45627400	-2.54745000	C	4.31790000	0.20352300	-1.79147500
H	0.10997200	3.88608800	-1.45816200	H	-1.51208400	3.47457800	-2.27984100
H	3.64233500	1.17343900	-1.90473100	H	4.00209600	-0.58092200	-2.47992500
H	-1.15301200	5.11538800	-1.50147500	H	0.08559900	3.80476400	-1.61274000
H	5.24747600	0.49076600	-2.17380300	H	3.68150400	1.07270900	-1.96140200
C	2.31445800	-2.87813500	-1.89716500	H	-1.14832700	5.06366100	-1.61020000
C	-2.96370500	1.19394700	-2.21927700	H	5.34183100	0.48397900	-2.05642600
H	3.20295900	-2.60831900	-2.47317100	C	2.36711000	-2.90931900	-1.89175100
H	-3.12031700	2.22674000	-2.53952700	C	-3.08841500	1.21197800	-2.12671500
H	1.47888300	-2.28222400	-2.26733100	H	3.24700000	-2.61976300	-2.47053000
H	-2.03220700	0.83685300	-2.65990000	H	-3.26531500	2.24368900	-2.43940000
H	2.09944500	-3.92920000	-2.11116900	H	1.51408300	-2.34683000	-2.27173300
H	-3.78043800	0.59985200	-2.63858500	H	-2.18481700	0.85489800	-2.62128900
C	3.72231800	-3.51065400	0.09921600	H	2.18577300	-3.96948700	-2.09164100
C	-4.26300400	1.63582400	-0.10578500	H	-3.92682000	0.61522300	-2.49621100
H	3.89869300	-3.38583300	1.16950200	C	3.78349300	-3.48765300	0.11183100
H	-4.31458300	1.51866100	0.97815300	C	-4.25972100	1.68118100	0.04973400
H	4.64507200	-3.26148600	-0.43068800	H	3.95186000	-3.35513500	1.18235000
H	-4.39083800	2.69542300	-0.34272200	H	-4.26581800	1.55256400	1.13320000
H	3.52995300	-4.57320400	-0.07730300	H	4.70092100	-3.21409000	-0.41515000
H	-5.12056400	1.10586200	-0.52994300	H	-4.37161900	2.74636800	-0.16961700
H	-0.65389400	-1.07345200	-0.11200800	H	3.62029900	-4.55525600	-0.06308100
H	0.02785600	-0.81838900	1.87584600	H	-5.14789700	1.17696400	-0.34155200
C	-0.85434700	-2.09412400	0.44291100	H	-0.63398500	-1.10977400	-0.08631600
C	-2.32539000	-2.38670000	0.18660700	H	-0.01081700	-0.79316900	1.91048500
C	-2.79596800	-2.62546100	-1.10468700	C	-0.87721000	-2.08794200	0.51892300
C	-4.13397000	-2.91978800	-1.32755000	C	-2.33765500	-2.38245100	0.21705600
C	-5.02060200	-2.98598200	-0.25653900	C	-2.76306700	-2.64352600	-1.08558800
C	-3.21384300	-2.46773200	1.25323600	C	-4.09248900	-2.94230000	-1.34927300
C	-4.55518200	-2.76336600	1.03328100	C	-5.01550100	-2.99121600	-0.30851500
H	-2.10623700	-2.57921000	-1.94334200	C	-3.26244200	-2.44488200	1.25370200
H	-4.48693800	-3.10510400	-2.33661500	C	-4.59522600	-2.74546600	0.99244400
H	-6.06525800	-3.22182500	-0.42809100	H	-2.04579600	-2.61094600	-1.90135800
H	-2.81870200	-2.32050400	2.25209200	H	-4.41047600	-3.14346800	-2.36683600
H	-5.23805300	-2.83034100	1.87397000	H	-6.05364600	-3.23017700	-0.51214300
H	5.86639000	1.03715900	0.17557300	H	-2.90417500	-2.27433000	2.26250300
H	4.27720700	1.66572400	0.58955200	H	-5.30677300	-2.79739200	1.81003700
H	5.00019400	0.36907200	1.55283300	H	5.75493000	1.18485000	0.29542900
H	-0.96697500	5.38892700	0.95982900	H	4.10935700	1.76419700	0.52379400
H	-1.27056000	4.06348100	2.07669600	H	4.79730400	0.57118300	1.63742800
H	0.23429300	4.11778000	1.14344300	H	-0.74938500	5.38999600	0.81841100
O	-0.47999300	-2.05199100	1.72476100	H	-1.03845500	4.11363400	1.99518600
H	-0.27879300	-2.79721600	-0.18765800	H	0.39968500	4.06458800	0.96001200
N	0.63274100	0.47804600	-1.88699600	O	-0.55950800	-1.96794300	1.81387000
C	1.62600100	2.01104600	-0.16650500	H	-0.27985700	-2.83764100	-0.03312400
2Cr-cis + PhCOCH₃-TS				2Cr-trans + PhCOCH₃-TS			
O	-2.15947100	2.98808400	0.30644500	O	2.01640000	2.83969400	-0.90143900
P	1.39160800	1.69335600	-0.14505500	P	-1.41023300	1.69556100	0.15397000
P	-2.62092100	-0.76017100	-0.004316800	P	2.65261000	-0.72974900	0.06945000
C	1.50637300	1.62076600	-2.00073600	C	-1.49829300	1.66285100	2.01324400
C	-2.65176500	-0.98153400	-1.89425000	C	2.70150700	-0.90087000	1.92690800
H	2.05674400	0.70465400	-2.23366500	H	-2.04883800	0.75594800	2.27909000
H	-2.10552000	-1.90283700	-2.11188600	H	2.18864100	-1.83341300	2.17758300
H	2.04988000	2.46332400	-2.43193100	H	-2.02999100	2.52012600	2.43115100
H	-3.66024700	-1.09946500	-2.29546600	H	3.71768000	-0.97221500	2.32112200
C	0.10967100	1.50896200	-2.58895700	C	-0.09169900	1.56270900	2.57774000

C	-1.93775000	0.18805300	-2.55433500	C	1.95886300	0.26643200	2.55730600
H	0.17393700	1.33720800	-3.67235400	H	-0.13730800	1.41335300	3.66563000
H	-1.83238500	0.00063000	-3.63188300	H	1.85737600	0.10196400	3.63915200
H	-0.45966900	2.42935200	-2.43580900	H	0.47285900	2.48025500	2.39568500
H	-2.51732200	1.10772900	-2.43973600	H	2.51837500	1.19479400	2.42093800
N	-0.61519900	0.39964100	-1.94415700	N	0.63242100	0.44579600	1.94407200
C	-2.81149000	-2.51946700	0.59418000	C	2.93827500	-2.50341000	-0.49740500
C	3.08035500	1.07797900	0.39188100	C	-3.12138300	1.09331300	-0.32883600
H	-1.85106800	-2.95555100	0.32233300	H	2.01623800	-2.98623800	-0.17465400
H	3.03412600	0.02233300	0.12036200	H	-3.08077800	0.04348500	-0.03305300
C	-4.30101700	-0.01150100	0.39802600	C	4.28960100	0.10430300	-0.36340700
C	1.49058800	3.52729800	0.30816200	C	-1.47120400	3.52663500	-0.29936700
C	-4.84235500	0.97662700	-0.63343400	C	4.67044500	1.24216000	0.58245300
C	0.82258300	4.46669000	-0.69394600	C	-0.63853600	4.41921100	0.61933200
O	-0.39564800	0.23709300	3.05474900	O	0.07068600	-0.32117000	-3.03932900
H	2.56272100	3.74991900	0.30404400	H	-2.52269700	3.80382500	-0.16661800
H	-4.98467700	-0.86655800	0.42671600	H	5.03906600	-0.68610800	-0.24824900
C	0.95879500	3.78361600	1.71962800	C	-1.09157200	3.76903800	-1.76199500
C	-4.27868100	0.62889700	1.78754900	C	4.31897100	0.58874000	-1.81484200
H	1.39945800	3.12044900	2.46382900	H	-1.64316300	3.13360900	-2.45370100
H	-3.87087300	-0.03123800	2.55261700	H	4.03149500	-0.18422400	-2.52641700
H	-0.12249300	3.65711900	1.76423400	H	-0.02818400	3.59993400	-1.92641300
H	-3.68601100	1.54304100	1.79089300	H	3.65607300	1.44082600	-1.95929700
H	1.18418700	4.81319400	2.01542700	H	-1.30650100	4.80972100	-2.02523700
H	-5.29811600	0.89397800	2.08512100	H	5.33386600	0.91079800	-2.06886100
C	-2.92072000	-2.57652100	2.11691800	C	3.01399700	-2.64686000	-2.01672700
C	3.26841800	1.15880300	1.90525400	C	-3.36853600	1.13807300	-1.83542700
H	-3.89859600	-2.23505800	2.46437200	H	3.97504200	-2.30392600	-2.40582200
H	3.40696800	2.18984900	2.24086200	H	-3.53901500	2.15907500	-2.18547100
H	-2.15298600	-1.97622400	2.60814500	H	2.22162600	-2.09701600	-2.52642700
H	2.42397000	0.73097400	2.44834800	H	-2.54124100	0.71199000	-2.40466200
H	-2.80463600	-3.61069400	2.45503700	H	2.91763500	-3.70198200	-2.28994100
H	4.16448900	0.60171200	2.19147800	H	-4.26571400	0.56032000	-0.07259200
C	-3.91585000	-3.33770600	-0.07057200	C	4.10689100	-3.21782800	0.17845100
C	4.25919400	1.70856900	-0.34532900	C	-4.26868600	1.75558100	0.43093400
H	-3.81930600	-3.36995700	-1.15760500	H	4.04403700	-3.19182900	1.26790400
H	4.18489900	1.59426700	-1.42822100	H	-4.16275500	1.66648900	1.51332200
H	-4.91189700	-2.95585000	0.16811300	H	5.07135100	-2.79572200	-0.11498900
H	4.36617100	2.77390000	-0.12279500	H	-4.36923700	2.81625700	0.18490600
H	-3.87670200	-4.37010800	0.29096200	H	4.11608900	-4.27013800	-0.12232800
H	5.18656300	1.22105900	-0.03010700	H	-5.21097400	1.27242800	0.15586900
H	0.31275600	-1.09924500	-0.06715300	H	-0.33335700	-1.09975300	0.06252300
H	-0.04579600	-0.44982800	-2.12173700	H	0.07061400	-0.40636200	2.14283800
C	1.15854400	-2.23330100	-1.09826800	C	-1.11717300	-2.18616000	1.08045200
C	2.46055600	-2.29590600	-0.33289700	C	-2.43383800	-2.28419000	0.33900000
C	2.52322800	-2.52552300	1.04140100	C	-2.51988900	-2.54139700	-1.02894900
C	3.74712600	-2.69601100	1.67070300	C	-3.75322900	-2.74264200	-1.63117600
C	4.92636200	-2.65081200	0.93257600	C	-4.91833800	-2.70185100	-0.87143100
C	3.64528000	-2.25110200	-1.06611000	C	-3.60512100	-2.24573100	1.09418700
C	4.87205500	-2.42736100	-0.43703600	C	-4.84069500	-2.45314900	0.49293200
H	1.60915000	-2.52966300	1.62443100	H	-1.61909600	-2.55184800	-1.63190900
H	3.78384600	-2.85957700	2.74223900	H	-3.80724800	-2.92799500	-2.69840300
H	5.88235200	-2.78957800	1.42561600	H	-5.88134000	-2.86504100	-1.34287600
H	3.58349400	-2.08251900	-2.13505200	H	-3.52420600	-2.05715200	2.15843800
H	5.78671000	-2.39529400	-1.01939700	H	-5.74410800	-2.42588900	1.09287100
H	-5.82910700	1.32592200	-0.31396800	H	5.64032400	1.64937300	0.28047800
H	-4.20516700	1.85704600	-0.72475400	H	3.95046100	2.06036300	0.54031400
H	-4.96458900	0.53042200	-1.62204800	H	4.76966600	0.91259300	1.61838300
H	0.97470300	5.50233500	-0.37406400	H	-0.76056200	5.46299400	0.31352200
H	1.23980000	4.37591000	-1.69849100	H	-0.94806600	4.35181700	1.66391800
H	-0.25436400	4.30357500	-0.74854600	H	0.42507300	4.18658300	0.55216000
O	1.13872400	-1.71223300	-2.23576900	O	-1.10163100	-1.67090200	2.22472000
N	-0.48731800	0.33181600	1.88560200	C	-0.23192500	-3.39727900	0.83152500

C -1.54891000	2.00076500	0.26199200	H -0.76026100	-4.26224000	1.24769100
C 0.28552200	-3.45016500	-0.84753700	H -0.05028700	-3.59181700	-0.22459300
H 0.81612500	-4.30572200	-1.28092200	H 0.70761300	-3.29265500	1.37024500
H 0.12735700	-3.65805800	0.20947800	C 0.28680600	-0.00417400	-1.94879300
H -0.66554700	-3.35291900	-1.36686100	N 1.43342600	1.85734100	-0.58100400
Cr -0.60173000	0.44515900	0.23293600	Cr 0.61258600	0.46972900	-0.20892700
1Mo-cis + H₂-TS			1Mo-trans + H₂-TS		
C 1.04981500	1.66546900	0.00000000	N -0.55320700	-1.75329800	0.00000000
O 1.76206600	2.57863900	0.00000000	O -1.01224100	-2.84351900	0.00000000
Mo -0.18870800	0.12453200	0.00000000	Mo 0.18573800	-0.10503800	0.00000000
P 0.01251500	-0.34728100	2.43752500	P -0.05755600	0.35272700	2.43604900
P 0.01251500	-0.34728100	-2.43752500	P -0.05755600	0.35272700	-2.43604900
C 1.12479900	-1.84463400	2.43983600	C -1.36050800	1.68943300	2.44444400
C 1.12479900	-1.84463400	-2.43983600	C -1.36050800	1.68943300	-2.44444400
H 0.46139500	-2.71417900	2.41597700	C -2.23389600	1.59397600	1.19865300
H 0.46139500	-2.71417900	-2.41597700	C -2.23389600	1.59397600	-1.19865300
H 1.71736500	-1.90806800	3.35548000	N -1.44038300	1.44321600	0.00000000
H 1.71736500	-1.90806800	-3.35548000	C 1.33226400	1.22172400	-3.36436900
C 2.01469200	-1.85741500	1.20156800	C 1.33226400	1.22172400	3.36436900
C 2.01469200	-1.85741500	-1.20156800	C -0.70426700	-0.98520000	-3.58106300
H 2.51413500	-2.83987300	1.14646600	C -0.70426700	-0.98520000	3.58106300
H 2.51413500	-2.83987300	-1.14646600	C -2.14961200	-1.35334700	-3.25156600
H 2.82246900	-1.11380400	1.32264100	C -2.14961200	-1.35334700	3.25156600
H 2.82246900	-1.11380400	-1.32264100	C 1.99888500	-0.92697400	0.00000000
N 1.24983700	-1.61316000	0.00000000	O 3.05673500	-1.39698800	0.00000000
C -1.51825900	-1.03977300	-3.28759600	H -0.67772200	-0.55566600	4.58855300
C -1.51825900	-1.03977300	3.28759600	H -0.67772200	-0.55566600	-4.58855300
H -1.72401200	-1.90593400	-2.64731400	C 0.18684000	-2.22576200	3.54082400
H -1.72401200	-1.90593400	2.64731400	C 0.18684000	-2.22576200	-3.54082400
C 0.78929500	0.84600000	-3.66142000	C 2.63538300	0.42876100	-3.41168000
C 0.78929500	0.84600000	3.66142000	C 2.63538300	0.42876100	3.41168000
C 2.27904800	1.04155400	-3.38914800	C 0.94073400	1.72630000	-4.75149800
C 2.27904800	1.04155400	3.38914800	C 0.94073400	1.72630000	4.75149800
N -1.60410100	1.26906200	0.00000000	H -0.81898300	2.64033100	2.43377200
O -2.53717200	1.99012800	0.00000000	H -0.81898300	2.64033100	-2.43377200
H 0.67756400	0.38197400	4.64726600	H -1.96336700	1.66560400	3.35539700
H 0.67756400	0.38197400	-4.64726600	H -1.96336700	1.66560400	-3.35539700
C 0.06072200	2.18848500	3.65306300	H -2.84868700	2.50902300	1.14081000
C 0.06072200	2.18848500	-3.65306300	H -2.84868700	2.50902300	-1.14081000
H -0.99015300	2.09847600	3.92941100	H -2.94695500	0.75832100	1.31393700
H -0.99015300	2.09847600	-3.92941100	H -2.94695500	0.75832100	-1.31393700
H 0.10638900	2.64990800	2.66437300	H 1.49782700	2.08924900	-2.71378500
H 0.10638900	2.64990800	-2.66437300	H 1.49782700	2.08924900	2.71378500
H 0.53322000	2.87172600	4.36503700	H 1.22030600	-2.01185800	3.81329900
H 0.53322000	2.87172600	-4.36503700	H 1.22030600	-2.01185800	-3.81329900
C -2.73284800	-0.11881500	-3.20648500	H 0.18933300	-2.67162200	2.54497700
C -2.73284800	-0.11881500	3.20648500	H 0.18933300	-2.67162200	-2.54497700
H -2.63982700	0.73658000	-3.87880600	H -0.19364600	-2.97410100	4.24261300
H -2.63982700	0.73658000	3.87880600	H -0.19364600	-2.97410100	-4.24261300
H -2.89018500	0.26057000	-2.19667700	H 2.58150100	-0.39011500	-4.13228700
H -2.89018500	0.26057000	2.19667700	H 2.58150100	-0.39011500	4.13228700
H -3.63135300	-0.66657400	-3.50626000	H 2.89688300	0.00926000	-2.44032400
H -3.63135300	-0.66657400	3.50626000	H 2.89688300	0.00926000	2.44032400
C -1.28204200	-1.53454000	-4.71212400	H 3.45346300	1.08192400	-3.72962100
C -1.28204200	-1.53454000	4.71212400	H 3.45346300	1.08192400	3.72962100
H -0.42634300	-2.20938100	-4.78573900	H 0.03217200	2.33138100	-4.73894400
H -0.42634300	-2.20938100	4.78573900	H 0.03217200	2.33138100	4.73894400
H -1.12007800	-0.70424300	-5.40401100	H 0.78870300	0.89996100	-5.45046000
H -1.12007800	-0.70424300	5.40401100	H 0.78870300	0.89996100	5.45046000
H -2.16200100	-2.07962000	-5.06718100	H 1.74342400	2.34742800	-5.16061500
H -2.16200100	-2.07962000	5.06718100	H 1.74342400	2.34742800	5.16061500
H -1.13614700	-1.61150800	0.00000000	H 0.94115600	1.76178900	0.00000000

H -0.23530400	-1.85421300	0.00000000	H 0.03869600	1.89022500	0.00000000
H 2.69484500	1.73564100	-4.12564700	H -2.48814200	-2.13821200	-3.93449400
H 2.69484500	1.73564100	4.12564700	H -2.48814200	-2.13821200	3.93449400
H 2.45153300	1.47052600	-2.40079900	H -2.24008500	-1.74054400	-2.23513800
H 2.45153300	1.47052600	2.40079900	H -2.24008500	-1.74054400	2.23513800
H 2.84435500	0.11086200	-3.46144700	H -2.83181200	-0.50855000	-3.35940400
H 2.84435500	0.11086200	3.46144700	H -2.83181200	-0.50855000	3.35940400
2Mo-cis + PhCN-TS-H_M transfer			2Mo-trans + PhCN-TS-H_M transfer		
C -2.72543900	0.59449700	0.00000000	C -0.17581700	-2.16028000	0.00000000
O -3.87016800	0.78939300	0.00000000	O 0.20487700	-3.25513600	0.00000000
Mo -0.75816400	0.30405700	0.00000000	Mo -0.79660100	-0.28242100	0.00000000
P -0.65661500	-0.18801700	-2.43434700	P -0.66424800	0.20699200	2.43350000
P -0.65661500	-0.18801700	2.43434700	P -0.66424800	0.20699200	-2.43350000
C -0.82038100	-2.04996300	-2.44802000	C -0.82978000	2.07143300	2.45446400
C -0.82038100	-2.04996300	2.44802000	C -0.82978000	2.07143300	-2.45446400
H 0.19802700	-2.44710200	-2.41280800	H 0.18728900	2.47333600	2.43434200
H 0.19802700	-2.44710200	2.41280800	H 0.18728900	2.47333600	-2.43434200
H -1.28266900	-2.41600800	-3.36674700	H -1.30751300	2.43387200	3.36716700
H -1.28266900	-2.41600800	3.36674700	H -1.30751300	2.43387200	-3.36716700
C -1.58206700	-2.54352300	-1.22657900	C -1.57766400	2.56217800	1.22353800
C -1.58206700	-2.54352300	1.22657900	C -1.57766400	2.56217800	-1.22353800
H -1.56043400	-3.64189800	-1.19869600	H -1.54869900	3.66045300	1.19046000
H -1.56043400	-3.64189800	1.19869600	H -1.54869900	3.66045300	-1.19046000
H -2.62961000	-2.23534100	-1.26245000	H -2.62754000	2.26130300	1.25365400
H -2.62961000	-2.23534100	1.26245000	H -2.62754000	2.26130300	-1.25365400
N -0.97648700	-1.99524800	0.00000000	N -0.97360000	2.00391900	0.00000000
C 0.97399200	0.04175200	3.34119400	C 0.94392600	-0.01476200	-3.38198800
C 0.97399200	0.04175200	-3.34119400	C 0.94392600	-0.01476200	3.38198800
H 1.66636000	-0.45061500	2.65008900	H 1.65005100	0.49262500	-2.71559200
H 1.66636000	-0.45061500	-2.65008900	H 1.65005100	0.49262500	2.71559200
C -1.96199300	0.45240900	3.63084600	C -2.01778200	-0.41715900	-3.57967300
C -1.96199300	0.45240900	-3.63084600	C -2.01778200	-0.41715900	3.57967300
C -3.28981800	-0.29086500	3.50583600	C -3.35102400	0.28660700	-3.33417600
C -3.28981800	-0.29086500	-3.50583600	C -3.35102400	0.28660700	3.33417600
N -0.40215900	2.08004900	0.00000000	N -2.53599500	-0.80786600	0.00000000
O -0.14088900	3.23221800	0.00000000	O -3.65354600	-1.20417600	0.00000000
C -2.17362400	1.95242600	-3.42648100	C -2.18618000	-1.93037100	3.44524300
C -2.17362400	1.95242600	3.42648100	C -2.18618000	-1.93037100	-3.44524300
H -1.25502900	2.52818900	-3.54097800	H -1.26263900	-2.47684300	3.63601100
H -1.25502900	2.52818900	3.54097800	H -1.26263900	-2.47684300	-3.63601100
H -2.56444300	2.15326600	-2.42726700	H -2.52685800	-2.19369800	2.44271500
H -2.56444300	2.15326600	2.42726700	H -2.52685800	-2.19369800	-2.44271500
H -2.89728400	2.32853600	-4.15603300	H -2.93597500	-2.28254000	4.16030400
H -2.89728400	2.32853600	4.15603300	H -2.93597500	-2.28254000	-4.16030400
C 1.37997000	1.51030000	3.43918700	C 1.37316500	-1.47561100	-3.48898300
C 1.37997000	1.51030000	-3.43918700	C 1.37316500	-1.47561100	3.48898300
H 0.79782400	2.03588700	4.20007600	H 0.78501800	-2.01141300	-4.23774500
H 0.79782400	2.03588700	-4.20007600	H 0.78501800	-2.01141300	4.23774500
H 1.25259500	2.03356400	2.49018200	H 1.27533000	-2.00100300	-2.53839500
H 1.25259500	2.03356400	-2.49018200	H 1.27533000	-2.00100300	2.53839500
H 2.43213800	1.58650100	3.72765000	H 2.42019300	-1.53191200	-3.79970000
H 2.43213800	1.58650100	-3.72765000	H 2.42019300	-1.53191200	3.79970000
C 1.06498300	-0.65097200	4.69831100	C 0.98208600	0.67411600	-4.74390000
C 1.06498300	-0.65097200	-4.69831100	C 0.98208600	0.67411600	4.74390000
H 0.82148700	-1.71390300	4.64565800	H 0.72409500	1.73325400	-4.68806900
H 0.82148700	-1.71390300	-4.64565800	H 0.72409500	1.73325400	4.68806900
H 0.40529500	-0.18752800	5.43644400	H 0.30646300	0.19652900	-5.45819000
H 0.40529500	-0.18752800	-5.43644400	H 0.30646300	0.19652900	5.45819000
H 2.08509000	-0.56933900	5.08591900	H 1.99062500	0.60586400	-5.16279600
H 2.08509000	-0.56933900	-5.08591900	H 1.99062500	0.60586400	5.16279600
H 1.02442400	-0.29866500	0.00000000	H 1.06397700	0.23911800	0.00000000
H 0.01732100	-2.29982900	0.00000000	H 0.02606700	2.29924600	0.00000000

N 1.84820000	-2.56739800	0.00000000	N 1.83562800	2.50638600	0.00000000
C 2.22593800	-1.44811800	0.00000000	C 2.20530200	1.38095200	0.00000000
C 3.40034900	-0.57849900	0.00000000	C 3.41031900	0.54839700	0.00000000
C 3.32287000	0.81013700	0.00000000	C 3.37923100	-0.84144200	0.00000000
C 4.48346700	1.57213600	0.00000000	C 4.56332100	-1.56680300	0.00000000
C 5.72666000	0.95315700	0.00000000	C 5.78582400	-0.90826200	0.00000000
C 4.65478000	-1.20228300	0.00000000	C 4.64433200	1.21144000	0.00000000
C 5.80875000	-0.43626500	0.00000000	C 5.82243000	0.48323400	0.00000000
H 2.34202100	1.27129500	0.00000000	H 2.41718700	-1.33843800	0.00000000
H 4.41341200	2.65402700	0.00000000	H 4.52762700	-2.65037800	0.00000000
H 6.63186800	1.55037900	0.00000000	H 6.70983500	-1.47593900	0.00000000
H 4.70369100	-2.28463600	0.00000000	H 4.65712000	2.29481500	0.00000000
H 6.77707500	-0.92429300	0.00000000	H 6.77449300	1.00237900	0.00000000
H -1.56396700	0.28126700	-4.63675900	H -1.68471600	-0.18224200	4.59652600
H -1.56396700	0.28126700	4.63675900	H -1.68471600	-0.18224200	-4.59652600
H -4.01051800	0.13080900	4.21285000	H -4.10414900	-0.11535700	-4.01847700
H -4.01051800	0.13080900	-4.21285000	H -4.10414900	-0.11535700	4.01847700
H -3.71533600	-0.18102300	2.50671900	H -3.71065700	0.11386500	-2.31818400
H -3.71533600	-0.18102300	-2.50671900	H -3.71065700	0.11386500	2.31818400
H -3.20148800	-1.35535900	3.73106000	H -3.29788400	1.36288100	-3.50852800
H -3.20148800	-1.35535900	-3.73106000	H -3.29788400	1.36288100	3.50852800
2Mo-cis + PhCN-interm			2Mo-trans + PhCN-interm		
C -0.00242200	-2.67985200	0.61837800	C -0.18829600	-2.16811500	0.00000000
O -0.00334100	-3.82054900	0.83501800	O 0.16221800	-3.27170100	0.00000000
Mo -0.00073700	-0.74747200	0.29281600	Mo -0.79305300	-0.27914700	0.00000000
P -2.44786200	-0.65256100	-0.19172000	P -0.65621500	0.20731200	2.44274300
P 2.44652800	-0.65713100	-0.19174000	P -0.65621500	0.20731200	-2.44274300
C -2.45244300	-0.74667500	-2.05473500	C -0.76481000	2.07272300	2.45576100
C 2.45095800	-0.75102400	-2.05476400	C -0.76481000	2.07272300	-2.45576100
H -2.41912200	0.28643900	-2.41135300	H 0.26460900	2.44118400	2.43514200
H 2.41960500	0.28218500	-2.41129300	H 0.26460900	2.44118400	-2.43514200
H -3.36652900	-1.20091700	-2.44202000	H -1.23383400	2.45241100	3.36593200
H 3.36421900	-1.20693200	-2.44204700	H -1.23383400	2.45241100	-3.36593200
C -1.22106700	-1.47864000	-2.56794000	C -1.49064100	2.58047000	1.21862400
C 1.21825100	-1.48067500	-2.56806800	C -1.49064100	2.58047000	-1.21862400
H -1.17897800	-1.39197200	-3.66259800	H -1.40800900	3.67555100	1.17482700
H 1.17629000	-1.39372100	-3.66270700	H -1.40800900	3.67555100	-1.17482700
H -1.26343900	-2.54378800	-2.32574500	H -2.55500800	2.33405800	1.25528200
H 1.25871700	-2.54594500	-2.32606800	H -2.55500800	2.33405800	-1.25528200
N -0.00088100	-0.89890200	-1.97621600	N -0.90938700	1.98704400	0.00000000
C 3.35603400	0.96110900	0.10318800	C 0.94348500	-0.06746300	-3.39139700
C -3.35460000	0.96724200	0.10302600	C 0.94348500	-0.06746300	3.39139700
H 2.67722300	1.67469900	-0.37641900	H 1.66814800	0.41922900	-2.72922900
H -2.67438500	1.67970200	-0.37628900	H 1.66814800	0.41922900	2.72922900
C 3.62266100	-1.99866200	0.40328300	C -2.03385600	-0.38315500	-3.57563700
C -3.62628700	-1.99199200	0.40357400	C -2.03385600	-0.38315500	3.57563700
C 3.46536800	-3.30207700	-0.37641300	C -3.34546400	0.35715900	-3.32102400
C -3.47118800	-3.29583700	-0.37581800	C -3.34546400	0.35715900	3.32102400
N -0.00050200	-0.39182200	2.07390400	N -2.51712400	-0.79784300	0.00000000
O -0.00020800	-0.13943900	3.22541400	O -3.64378200	-1.16437800	0.00000000
C -3.44154600	-2.24080300	1.90025500	C -2.24093900	-1.89173600	3.44434500
C 3.43744300	-2.24747300	1.89990800	C -2.24093900	-1.89173600	-3.44434500
H -3.57600600	-1.33931300	2.49809900	H -1.33193100	-2.46134100	3.63677400
H 3.57378900	-1.34640900	2.49796800	H -1.33193100	-2.46134100	-3.63677400
H -2.44233300	-2.62788900	2.10748000	H -2.58962100	-2.14964900	2.44326100
H 2.43741400	-2.63252300	2.10703900	H -2.58962100	-2.14964900	-2.44326100
H -4.16891300	-2.98182000	2.24516900	H -2.99936800	-2.22218600	4.16052400
H 4.16326300	-2.99008600	2.24463600	H -2.99936800	-2.22218600	-4.16052400
C 3.44386100	1.32440100	1.58356700	C 1.32845900	-1.54035800	-3.50158500
C -3.44227200	1.33047800	1.58342000	C 1.32845900	-1.54035800	3.50158500
H 4.19658800	0.72334300	2.09927200	H 0.72211900	-2.05776000	-4.24870600
H -4.19589300	0.73036500	2.09891800	H 0.72211900	-2.05776000	4.24870600

H 2.49019800	1.19114000	2.09672100	H 1.22087100	-2.06507300	-2.55165100
H -2.48888200	1.19592800	2.09675900	H 1.22087100	-2.06507300	2.55165100
H 3.73814300	2.37211500	1.68991900	H 2.37213700	-1.62586500	-3.81624000
H -3.73520300	2.37856800	1.68982200	H 2.37213700	-1.62586500	3.81624000
C 4.71963800	1.06201700	-0.57582000	C 0.99699500	0.62197700	-4.75272700
C -4.71781200	1.07060500	-0.57637800	C 0.99699500	0.62197700	4.75272700
H 4.67383900	0.84923000	-1.64555800	H 0.77347900	1.68865900	-4.69396000
H -4.67209500	0.85787100	-1.64612500	H 0.77347900	1.68865900	4.69396000
H 5.44949900	0.38502300	-0.12438800	H 0.30380500	0.16668800	-5.46477100
H -5.44901000	0.39486600	-0.12522800	H 0.30380500	0.16668800	5.46477100
H 5.11176000	2.07712100	-0.46234600	H 2.00134000	0.52237800	-5.17498300
H -5.10816000	2.08639600	-0.46290800	H 2.00134000	0.52237800	5.17498300
H 0.00164500	1.14988700	-0.39401500	H 1.16567600	0.33800500	0.00000000
H -0.00008200	0.14366000	-2.27802500	H 0.13018100	2.27343400	0.00000000
N 0.00105300	1.77236400	-2.45868200	N 1.78107900	2.42552700	0.00000000
C 0.00188600	2.05540500	-1.27627600	C 2.07173300	1.24746700	0.00000000
C 0.00331400	3.33573100	-0.52820100	C 3.35813800	0.50924700	0.00000000
C 0.00351100	3.36159400	0.86235600	C 3.40474600	-0.88032300	0.00000000
C 0.00479500	4.57208400	1.54433000	C 4.62485700	-1.54509700	0.00000000
C 0.00592500	5.76695200	0.83629900	C 5.80955800	-0.82054800	0.00000000
C 0.00444700	4.54008800	-1.23738100	C 4.55297400	1.23515900	0.00000000
C 0.00575000	5.74665700	-0.55649200	C 5.76909500	0.57175200	0.00000000
H 0.00264200	2.42050400	1.40424700	H 2.47377800	-1.43744400	0.00000000
H 0.00492600	4.58139900	2.62879600	H 4.64890600	-2.62930000	0.00000000
H 0.00695100	6.71331200	1.36612100	H 6.76331400	-1.33689900	0.00000000
H 0.00425700	4.50093200	-2.32073100	H 4.49861700	2.31778200	0.00000000
H 0.00663000	6.67863500	-1.11154100	H 6.69281400	1.14042200	0.00000000
H -4.63506100	-1.60335700	0.22795300	H -1.70023300	-0.15481400	4.59377100
H 4.63208400	-1.61171100	0.22772500	H -1.70023300	-0.15481400	-4.59377100
H 4.16935600	-4.04419900	0.01157900	H -4.11287200	-0.02199800	-4.00234800
H -4.17632000	-4.03673700	0.01242900	H -4.11287200	-0.02199800	4.00234800
H 2.46246000	-3.71726100	-0.26214500	H -3.70499100	0.19261100	-2.30362600
H -2.46892400	-3.71259600	-0.26155600	H -3.70499100	0.19261100	2.30362600
H 3.67325500	-3.18435800	-1.44138700	H -3.26245900	1.43178500	-3.49287000
H -3.67899200	-3.17805400	-1.44080100	H -3.26245900	1.43178500	3.49287000
2Mo-cis + PhCN-TS-H_N transfer			2Mo-trans + PhCN-TS-H_N transfer		
C 2.69819100	-0.59562400	0.00000000	C 0.21488200	-2.16244100	0.00000000
O 3.84131700	-0.79908900	0.00000000	O -0.14038900	-3.26463200	0.00000000
Mo 0.77497300	-0.28421600	0.00000000	Mo 0.82229600	-0.27050700	0.00000000
P 0.67455300	0.18871800	-2.45143800	P 0.67796100	0.20309300	-2.44745200
P 0.67455300	0.18871800	2.45143800	P 0.67796100	0.20309300	2.44745200
C 0.64505100	2.05130900	-2.45683200	C 0.63838300	2.06788200	-2.46194000
C 0.64505100	2.05130900	2.45683200	C 0.63838300	2.06788200	2.46194000
H -0.40970000	2.33813800	-2.44787900	H -0.41683600	2.35343900	-2.47159500
H -0.40970000	2.33813800	2.44787900	H -0.41683600	2.35343900	2.47159500
H 1.09245800	2.46745700	-3.36178500	H 1.10030500	2.48183700	-3.36099100
H 1.09245800	2.46745700	3.36178500	H 1.10030500	2.48183700	3.36099100
C 1.31543900	2.60660100	-1.20797100	C 1.28946300	2.62679700	-1.20495400
C 1.31543900	2.60660100	1.20797100	C 1.28946300	2.62679700	1.20495400
H 1.12010900	3.68777000	-1.15284300	H 1.07600400	3.70461900	-1.14653400
H 1.12010900	3.68777000	1.15284300	H 1.07600400	3.70461900	1.14653400
H 2.40245800	2.48151200	-1.25924700	H 2.37892600	2.52053500	-1.24956400
H 2.40245800	2.48151200	1.25924700	H 2.37892600	2.52053500	1.24956400
N 0.79198200	1.94818800	0.00000000	N 0.77569200	1.95509400	0.00000000
C -0.91843600	-0.21500800	3.36550000	C -0.88520800	-0.19929100	3.41355300
C -0.91843600	-0.21500800	-3.36550000	C -0.88520800	-0.19929100	-3.41355300
H -1.66104500	0.24513800	2.70418400	H -1.64959100	0.25608700	2.77369500
H -1.66104500	0.24513800	-2.70418400	H -1.64959100	0.25608700	-2.77369500
C 2.06024600	-0.31372700	3.61727400	C 2.11392100	-0.27587800	3.55772000
C 2.06024600	-0.31372700	-3.61727400	C 2.11392100	-0.27587800	-3.55772000
C 3.31835400	0.52884600	3.41843800	C 3.36936400	0.53640600	3.24497500

C	3.31835400	0.52884600	-3.41843800	C	3.36936400	0.53640600	-3.24497500
N	0.44429000	-2.07483400	0.00000000	N	2.53611200	-0.79452700	0.00000000
O	0.20036200	-3.22833400	0.00000000	O	3.66870800	-1.14312200	0.00000000
C	2.38273500	-1.79983800	-3.46538600	C	2.40966000	-1.77246300	-3.46605100
C	2.38273500	-1.79983800	3.46538600	C	2.40966000	-1.77246300	3.46605100
H	1.51694600	-2.43955100	-3.63669200	H	1.54423000	-2.38954500	-3.70693700
H	1.51694600	-2.43955100	3.63669200	H	1.54423000	-2.38954500	3.70693700
H	2.75918100	-2.01443700	-2.46374900	H	2.74397500	-2.04287900	-2.46348800
H	2.75918100	-2.01443700	2.46374900	H	2.74397500	-2.04287900	2.46348800
H	3.15623500	-2.08605500	-4.18431600	H	3.20860200	-2.03181100	-4.16727900
H	3.15623500	-2.08605500	4.18431600	H	3.20860200	-2.03181100	4.16727900
C	-1.21069600	-1.71266600	3.42002700	C	-1.18108100	-1.69438900	3.49778000
C	-1.21069600	-1.71266600	-3.42002700	C	-1.18108100	-1.69438900	-3.49778000
H	-0.58315500	-2.21697100	4.15848600	H	-0.53852700	-2.18950700	4.22929500
H	-0.58315500	-2.21697100	-4.15848600	H	-0.53852700	-2.18950700	-4.22929500
H	-1.05664100	-2.19748500	2.45484200	H	-1.05163100	-2.19479700	2.53763900
H	-1.05664100	-2.19748500	-2.45484200	H	-1.05163100	-2.19479700	-2.53763900
H	-2.25085000	-1.87536800	3.71584800	H	-2.21460500	-1.84753000	3.82067000
H	-2.25085000	-1.87536800	-3.71584800	H	-2.21460500	-1.84753000	-3.82067000
C	-1.04240100	0.42741900	4.74492000	C	-0.96048100	0.45842500	4.78971800
C	-1.04240100	0.42741900	-4.74492000	C	-0.96048100	0.45842500	-4.78971800
H	-0.87492300	1.50602100	4.72303300	H	-0.79804100	1.53708600	4.75069700
H	-0.87492300	1.50602100	-4.72303300	H	-0.79804100	1.53708600	-4.75069700
H	-0.34303300	-0.01179500	5.46087200	H	-0.23281700	0.02862200	5.48284100
H	-0.34303300	-0.01179500	-5.46087200	H	-0.23281700	0.02862200	-5.48284100
H	-2.04974300	0.26164100	5.13848400	H	-1.95169200	0.29316600	5.22234600
H	-2.04974300	0.26164100	-5.13848400	H	-1.95169200	0.29316600	-5.22234600
H	-1.23852400	0.29717400	0.00000000	H	-1.26312500	0.26088600	0.00000000
H	-0.39739000	2.23035000	0.00000000	H	-0.42711400	2.21719100	0.00000000
N	-1.76440900	2.34419300	0.00000000	N	-1.78345400	2.31337800	0.00000000
C	-2.07845300	1.15427900	0.00000000	C	-2.10025700	1.12411700	0.00000000
C	-3.40197200	0.49140300	0.00000000	C	-3.42983100	0.47279200	0.00000000
C	-3.50208300	-0.89735700	0.00000000	C	-3.54840800	-0.91436800	0.00000000
C	-4.74722800	-1.51362000	0.00000000	C	-4.80146000	-1.51460700	0.00000000
C	-5.90197800	-0.74181900	0.00000000	C	-5.94623100	-0.72833800	0.00000000
C	-4.56658600	1.26353000	0.00000000	C	-4.58499300	1.25940600	0.00000000
C	-5.80762500	0.64805000	0.00000000	C	-5.83382200	0.66016000	0.00000000
H	-2.59367900	-1.49273500	0.00000000	H	-2.65020600	-1.52387200	0.00000000
H	-4.81534200	-2.59592900	0.00000000	H	-4.88292400	-2.59596300	0.00000000
H	-6.87535600	-1.22013300	0.00000000	H	-6.92562100	-1.19418700	0.00000000
H	-4.46919500	2.34323400	0.00000000	H	-4.47371200	2.33773000	0.00000000
H	-6.70901700	1.25142300	0.00000000	H	-6.72722500	1.27529000	0.00000000
H	1.68072400	-0.13202900	-4.62841100	H	1.79275500	-0.03629300	-4.57728500
H	1.68072400	-0.13202900	4.62841100	H	1.79275500	-0.03629300	4.57728500
H	4.09226300	0.19525200	4.11606500	H	4.17865300	0.22215400	3.91069600
H	4.09226300	0.19525200	-4.11606500	H	4.17865300	0.22215400	-3.91069600
H	3.72037400	0.41559500	2.41016200	H	3.70730400	0.36991700	2.22057700
H	3.72037400	0.41559500	-2.41016200	H	3.70730400	0.36991700	-2.22057700
H	3.14806900	1.59038500	3.60598900	H	3.22405400	1.60773600	3.39375400
H	3.14806900	1.59038500	-3.60598900	H	3.22405400	1.60773600	-3.39375400
2Mo-cis + PhCHNH-TS				2Mo-trans + PhCHNH-TS			
N	-0.59004900	0.57223800	1.99429000	N	-0.60701900	0.57255800	2.00060900
H	0.58689900	-0.98960800	0.23537600	H	0.62507200	-0.99862500	0.19655700
H	0.00157600	-0.26509900	2.27012600	H	-0.02947600	-0.28526500	2.26487100
C	1.03398800	-2.08093200	1.22409200	C	1.00976000	-2.06922700	1.15613300
N	1.04720900	-1.64348100	2.47268700	N	0.97272500	-1.67031500	2.42365000
C	2.25212700	-2.56134100	0.48666600	C	2.26269600	-2.54240200	0.46739100
C	2.21161700	-2.78426000	-0.89076200	C	2.26162300	-2.80818800	-0.90284900
C	3.30988500	-3.30148300	-1.55942500	C	3.39028800	-3.30949300	-1.53204300
C	4.47553700	-3.60326900	-0.86095400	C	4.54797600	-3.55423400	-0.79923600
C	4.52618200	-3.39009500	0.50937400	C	4.55911700	-3.30100600	0.56514400
C	3.41904300	-2.87969100	1.17917200	C	3.42180400	-2.80549700	1.19446300

P -2.53551800	-0.92548800	0.16664100	P -2.55536400	-0.91661700	0.19124800
P 1.52057400	1.80869300	0.16785000	P 1.51115800	1.80459200	0.18689700
N -0.36710200	0.23707500	-2.08888600	C 3.20789600	1.06396800	-0.12689300
C -1.63021900	2.11684400	-0.54141800	C -2.59912000	-2.76770300	-0.15424000
C 3.19688000	1.02443300	-0.14547200	C 1.63573600	3.59784400	-0.36442400
C -2.51657900	-2.76645700	-0.22670000	C -4.25112700	-0.29030600	-0.32699000
C 1.71355000	3.58773000	-0.41929100	O -2.11407300	2.88912600	-1.21975200
C -4.26492000	-0.37519400	-0.34017100	C -2.58461600	-0.90198500	2.06091300
O -2.25702800	3.07952700	-0.71457500	C 1.48900200	1.87443200	2.05630500
C -2.53372100	-0.93718900	2.03418600	H -1.99925600	-1.76550700	2.39083000
C 1.48862900	1.88822100	2.03433800	H 2.08392200	1.02431100	2.40174400
H -1.91410100	-1.78562500	2.33957900	H -3.59536600	-1.01733100	2.45907700
H 2.08122800	1.03800300	2.38265000	H 1.96345700	2.77915300	2.44259300
H -3.53214600	-1.09519100	2.44742500	C -1.93662000	0.36443100	2.60289100
H 1.96517700	2.79243700	2.41776300	C 0.07087400	1.74033300	2.59124400
C -1.91849900	0.34050500	2.58875200	H -1.84259000	0.28276100	3.69499900
C 0.07036500	1.75644700	2.57075100	H 0.10184800	1.64224300	3.68606000
H -1.82903900	0.25560900	3.68073400	H -2.55291300	1.24194400	2.39200000
H 0.10039900	1.67366900	3.66660900	H -0.51675500	2.63271000	2.36085300
H -2.55222100	1.20535600	2.37738500	H 3.09315400	0.07002600	0.31927300
H -0.52256800	2.64161900	2.32668600	H -1.68849800	-3.10346600	0.35327000
H 3.05720400	0.03498700	0.30286400	C 0.68340100	4.50925200	0.40746700
H -1.56006200	-3.07303100	0.20836000	C -4.67839500	0.94990900	0.45534500
C 0.87981400	4.57667300	0.39224000	O 0.03007300	-0.35079000	-3.24104700
C -4.80774500	0.75557600	0.53037400	H -4.94973800	-1.09959100	-0.08973400
O -0.24440900	0.04698900	-3.24653500	H 2.66341100	3.90586800	-0.14221500
H -4.90844500	-1.25024300	-0.20195700	C -4.29948600	-0.01700600	-1.83000700
H 2.77137200	3.83476100	-0.27937900	C 1.39161500	3.72671600	-1.86808800
C -4.28921000	0.02879400	-1.81413500	H -4.03124400	-0.88927200	-2.42600900
C 1.37176400	3.69840000	-1.90528500	H 2.05946500	3.10056300	-2.45915000
H -3.93485800	-0.76235900	-2.47500800	H -3.62167500	0.79318000	-2.10114100
H 1.96050500	3.02228600	-2.52531900	H 0.36662700	3.45257600	-2.12066100
H -3.66338100	0.90570400	-1.98613800	H -5.31253700	0.28203700	-2.11598800
H 0.31881100	3.47044700	-2.07858800	H 1.54729700	4.76491300	-2.17719500
H -5.31168700	0.27995900	-2.11220700	C 3.50361300	0.86461300	-1.61113000
H 1.55792200	4.71908900	-2.25310500	C -2.44930900	-3.10449200	-1.63570700
C 3.46641800	0.81593900	-1.63369200	H 3.75288200	1.80920700	-2.10046900
C -2.44447300	-3.04061600	-1.72726300	H -3.37594800	-2.92199200	-2.18418200
H 3.71552500	1.75626500	-2.13178300	H 2.66187700	0.41461800	-2.13828000
H -3.40781900	-2.86766000	-2.21239700	H -1.65588500	-2.52468200	-2.10906500
H 2.61003100	0.37165100	-2.14321400	H 4.36431500	0.20077700	-1.72730400
H -1.69716400	-2.41776000	-2.22202000	H -2.21074700	-4.16561500	-1.75241200
H 4.31824700	0.14314300	-1.76312700	C 4.35830400	1.78290100	0.57370200
H -2.18089500	-4.08792800	-1.90118600	C -3.77872900	-3.50838300	0.47118900
C 4.37353100	1.71233600	0.54171200	H 4.19526100	1.89768600	1.64708900
C -3.61894800	-3.58523300	0.44016300	H -3.88114200	-3.30922300	1.53967900
H 4.22094500	1.83869400	1.61559300	H 4.53435700	2.77495300	0.14976600
H -3.65898600	-3.43375600	1.52060800	H -4.72249500	-3.25084900	-0.01574300
H 4.57780200	2.69616600	0.11125400	H 5.28152600	1.21054500	0.44334300
H -4.60406700	-3.35391300	0.02752900	H -3.64157300	-4.58736300	0.35179300
H 5.27808800	1.11122000	0.40926000	H 1.36824100	-2.59628600	-1.48065900
H -3.44276400	-4.65118300	0.26624800	H 3.37007400	-3.50544900	-2.59855100
H 1.31375500	-2.51852100	-1.43893400	H 5.43232700	-3.94553400	-1.28996100
H 3.26096900	-3.46351100	-2.63072400	H 3.42722700	-2.65277600	2.26813200
H 5.33619200	-4.00603800	-1.38355200	H 5.45074200	-3.50374300	1.14871400
H 3.45157900	-2.75742700	2.25636400	H -5.66562200	1.27129800	0.11016000
H 5.42465100	-3.63561400	1.06534400	H 0.79213700	5.53600000	0.04548200
H -5.80840800	1.03097500	0.18407500	H -4.75662100	0.76220200	1.52782500
H 1.03172000	5.58662000	-0.00030900	H 0.88828700	4.52163400	1.47963200
H -4.89566600	0.47342400	1.58118300	H -3.99141900	1.78218800	0.29398800
H 1.15610800	4.59635400	1.44810100	H -0.35767700	4.22003800	0.25340500
H -4.18512300	1.64896800	0.46032700	H 0.15040900	-2.66837600	0.85098600
H -0.18667200	4.35840000	0.31613600	H 1.89162200	-1.33698200	2.71405900

H 0.15240400 -2.66544100 0.96075000	C -0.19375100 -0.02142700 -2.15356200
H 1.97781700 -1.30339000 2.71566500	N -1.52027600 1.94631800 -0.81235400
Mo -0.53370800 0.48808700 -0.30080200	Mo -0.55677600 0.50833300 -0.28115900
2Mo-cis + PhCHNCH₂Ph-TS	2Mo-trans + PhCHNCH₂Ph-TS
O -2.81102800 0.36015100 2.82489700	C -2.10089700 0.21059100 1.99348300
Mo -1.30070000 0.55698100 0.24935300	O -2.53870900 0.00748500 3.04553500
P 0.45104500 2.20367000 0.89168100	P 0.35757800 2.28155800 0.79427500
P -2.50871000 -1.15273000 -1.11287600	P -2.45156200 -1.26330100 -1.11302800
C 1.52426700 2.21180100 -0.63774900	C 1.44661800 2.27840000 -0.72652700
C -1.38148400 -1.26395300 -2.60079500	C -1.33078600 -1.36590800 -2.60962500
H 2.32277200 1.48718500 -0.46744900	H 2.27908700 1.60103300 -0.52510400
H -0.63589900 -2.03189200 -2.37532000	H -0.56909400 -2.11916900 -2.38699700
H 2.00492100 3.17836100 -0.79792700	H 1.87913100 3.26139100 -0.92417200
H -1.91413700 -1.58708900 -3.49775500	H -1.86606000 -1.70120600 -3.50140800
C 0.73681800 1.79827800 -1.87277200	C 0.68319900 1.77969600 -1.94441000
C -0.66852200 0.05841900 -2.85300500	C -0.64966200 -0.02979500 -2.87550400
H 1.42531800 1.69203600 -2.72180200	H 1.38052000 1.66150500 -2.78490600
H 0.05487700 -0.06754200 -3.67014800	H 0.09036000 -0.15261400 -3.67841000
H -0.00083500 2.56000700 -2.13786500	H -0.07970300 2.50155400 -2.24658800
H -1.37862500 0.82914900 -3.16159100	H -1.37583700 0.71321800 -3.21251700
N 0.02359300 0.52770600 -1.63793300	N 0.00834200 0.49657400 -1.66396800
C -2.62107800 -2.94804400 -0.55244200	C -2.51969700 -3.06955300 -0.57367300
C 1.68633900 1.78434800 2.24578700	C 1.61869400 2.01982300 2.16524200
H -1.60308600 -3.15004100 -0.20776400	H -1.46100300 -3.29510000 -0.41147700
H 1.93999300 0.74941200 1.99544300	H 1.95364100 0.99873900 1.95506200
C -4.23247300 -0.81451300 -1.79989500	C -4.16056300 -0.92635900 -1.82475200
C 0.01937700 4.00692000 1.23612700	C -0.19032500 4.07170800 0.98846500
C -4.23162500 0.13657300 -2.99436300	C -4.15285400 0.16977000 -2.88818100
C -0.22076600 4.82633400 -0.02989400	C -0.60429200 4.70611100 -0.33819300
O -3.14466800 2.85924300 -0.82443200	N -2.60640800 1.76864000 -0.17385800
C -1.18983300 4.10198900 2.16706500	O -3.46128300 2.57383700 -0.34439300
C -5.15851800 -0.28800800 -0.70314400	C -1.31970800 4.19950800 2.01136300
H -1.06143000 3.53265700 3.08761400	C -5.16240800 -0.59370800 -0.71923600
H -5.19831000 -0.94208500 0.16759200	H -1.06639700 3.76661500 2.97855900
H -2.08932900 3.73053200 1.67451700	H -5.22739900 -1.37375500 0.03918400
H -4.83596000 0.69567500 -0.36060600	H -2.22671500 3.71117300 1.65433100
H -1.36324100 5.14713800 2.44123600	H -4.89884700 0.33834400 -0.21850200
H -6.17555200 -0.19094000 -1.09528300	H -1.54983300 5.25756100 2.17055800
C -3.54159900 -3.11451500 0.65522600	H -6.15904700 -0.47056500 -1.15401000
C 1.03688800 1.77586800 3.62775500	C -3.22939200 -3.26622200 0.76374700
H -4.59390300 -3.03873600 0.37168800	C 0.98828800 2.01840300 3.55591500
H 0.84744700 2.79037200 3.98679600	H -4.31342000 -3.18408800 0.66118500
H -3.33788200 -2.37289200 1.42965200	H 0.75427200 3.03211600 3.88889200
H 0.09139200 1.23027700 3.63343400	H -2.90074900 -2.54127200 1.50899900
H -3.39674500 -4.10555300 1.09455800	H 0.07126600 1.42821100 3.59241400
H 1.70615600 1.29735600 4.34824600	H -3.01733700 -4.26727900 1.14997100
C -2.95631300 -3.95035400 -1.65399800	H 1.69135800 1.59573200 4.27915700
C 2.96385200 2.61950700 2.23901600	C -3.03958100 -4.03693300 -1.63441200
H -2.27029000 -3.88883100 -2.50096500	C 2.82830300 2.94965600 2.11013800
H 3.47781800 2.59525700 1.27626200	H -2.53134500 -3.92276600 -2.59425700
H -3.97351800 -3.81821700 -2.03125300	H 3.33523600 2.92616000 1.14389200
H 2.76811900 3.66492800 2.49135700	H -4.11278600 -3.91741200 -1.80081900
H -2.89336100 -4.96791500 -1.25637400	H 2.55291100 3.98565900 2.32345300
H 3.65951500 2.23488800 2.99119700	H -2.88140700 -5.06713000 -1.30142300
H 0.03733800 -0.78896200 0.63091300	H 3.55724400 2.65047500 2.86946300
H 0.74930200 -0.19485700 -1.41195000	H 0.07511500 -0.73947600 1.73557800
N 1.86086100 -1.54298900 -0.74587800	H 0.75556400 -0.19654400 -1.40528600
H 0.89218700 4.42317000 1.75052500	N 1.87601500 -1.46761800 -0.67053000
H -4.60729700 -1.78576000 -2.13960800	H 0.68938300 4.60674500 1.36303400
H -5.25911400 0.28208000 -3.34106600	H -4.46327000 -1.86138600 -2.30728400
H -0.46622800 5.85594500 0.24736000	H -5.17201700 0.31841500 -3.25743400
H -3.84183300 1.11931700 -2.72411300	H -0.90614400 5.74307700 -0.16305700

H -1.06314200	4.43909500	-0.60514500	H -3.81341100	1.12346200	-2.48180500
H -3.65714600	-0.24648500	-3.83979200	H -1.45949200	4.19055400	-0.77791800
H 0.65472100	4.86813600	-0.68018900	H -3.53306900	-0.08697500	-3.74933500
C 3.15108400	-1.11162700	-0.25963900	H 0.20688100	4.72540300	-1.06817700
H 3.06430200	-0.32046700	0.50347900	C 3.16260600	-0.99728500	-0.21323000
H 3.67597500	-1.92818300	0.25834500	H 3.07005100	-0.15799500	0.49693000
C 4.05514200	-0.61297900	-1.36378900	H 3.69311800	-1.77523500	0.35685900
C 3.81620100	-0.92631000	-2.69950600	C 4.06202300	-0.56197800	-1.34722300
C 5.18285000	0.14761800	-1.05047100	C 3.83290600	-0.97368900	-2.65776200
C 4.68164100	-0.48931100	-3.69668200	C 5.17536400	0.23849600	-1.08668300
H 2.94162300	-1.51945800	-2.93796500	C 4.69448400	-0.59495500	-3.68161200
C 6.04827300	0.58587100	-2.04353900	H 2.96845100	-1.59596200	-2.85550900
H 5.38675100	0.39733300	-0.01279400	C 6.03711300	0.61878000	-2.10653600
C 5.79987600	0.26861800	-3.37444500	H 5.37091500	0.56598400	-0.06921000
H 4.48215600	-0.74587600	-4.73205200	C 5.79903000	0.20258800	-3.41176600
H 6.91872100	1.17678400	-1.77889900	H 4.50275800	-0.92796500	-4.69648400
H 6.47395600	0.60970500	-4.15249900	H 6.89648600	1.24197400	-1.88291400
C 0.97677500	-1.96088100	0.13748200	H 6.47022800	0.49823700	-4.21063700
H 0.11834700	-2.44855200	-0.31961300	C 1.01317500	-1.87661500	0.24220500
C 1.32093300	-2.57412100	1.47220900	H 0.16290600	-2.40484800	-0.18434700
C 2.13665300	-3.71120100	1.46378500	C 1.41289800	-2.45801700	1.57688300
C 0.81444000	-2.12988400	2.68977400	C 2.17057900	-3.63446900	1.55444600
C 2.44549300	-4.37354400	2.64321400	C 1.03637600	-1.93511900	2.80929700
H 2.52217300	-4.07993300	0.51891600	C 2.54462200	-4.26180200	2.73388600
C 1.12067600	-2.79492600	3.87211400	H 2.46395700	-4.05692300	0.59892400
H 0.17034600	-1.25853000	2.69757000	C 1.40808700	-2.56459100	3.99266900
C 1.93957100	-3.91543200	3.85458400	H 0.43921100	-1.03203700	2.83388300
H 3.07920100	-5.25350100	2.61553000	C 2.16437400	-3.72756600	3.96015300
H 0.71355700	-2.43339200	4.81025000	H 3.13110100	-5.17352100	2.69544500
H 2.18017400	-4.43211400	4.77720700	H 1.09973600	-2.14258700	4.94307300
N -2.22533000	0.44715000	1.80505000	H 2.45496300	-4.21745000	4.88296400
C -2.45764400	2.00338000	-0.44287700	Mo -1.32521100	0.54515500	0.20351000
2Mo-cis + PhCHNPh-TS			2Mo-trans + PhCHNPh-TS		
O -1.95305300	0.22434800	3.21727400	O -1.56430000	-0.02330800	3.37970000
Mo -1.20415700	0.46610600	0.33161500	Mo -1.23052900	0.45671000	0.30024000
P 0.38386400	2.37618600	0.42404700	P 0.32165800	2.39423500	0.34852500
P -2.46237300	-1.48296900	-0.60513200	P -2.43004600	-1.55650800	-0.60669300
C 1.05745800	2.36543900	-1.31764900	C 1.00962500	2.35222800	-1.38976300
C -1.80089000	-1.51626500	-2.35434600	C -1.82010600	-1.58627500	-2.37717400
H 1.94168400	1.72242200	-1.30238600	H 1.91474400	1.73957100	-1.35471100
H -0.91797500	-2.16268300	-2.34444800	H -0.94225100	-2.23887100	-2.40184400
H 1.38641300	3.35586600	-1.63831600	H 1.30608800	3.34433100	-1.73808500
H -2.51317500	-1.95421900	-3.05649900	H -2.56207200	-2.00762400	-3.05994200
C 0.03996600	1.80087200	-2.30027900	C 0.01445400	1.73069600	-2.35919900
C -1.38506800	-0.12463600	-2.81444800	C -1.41016300	-0.19207600	-2.83292500
H 0.49984000	1.71644900	-3.29441400	H 0.48949600	1.61175400	-3.34273100
H -0.91769500	-0.19346100	-3.80648100	H -0.94278900	-0.25646900	-3.82555200
H -0.82261600	2.46549200	-2.39339400	H -0.85453300	2.37972400	-2.49165500
H -2.25312800	0.53219500	-2.90528700	H -2.27979900	0.46277600	-2.92198900
N -0.44461100	0.48068900	-1.85388500	N -0.47373500	0.42484200	-1.87366600
C -2.14925600	-3.24988400	-0.02719700	C -2.08196200	-3.33456200	-0.07016800
C 1.94386800	2.22242700	1.45610700	C 1.89275800	2.35727600	1.37731100
H -1.05699400	-3.30151400	-0.00011000	H -1.05834300	-3.48385600	-0.42946000
H 2.28748600	1.22838400	1.15763400	H 2.28372200	1.37055500	1.11292400
C -4.34173200	-1.42503500	-0.76392100	C -4.30216100	-1.47912300	-0.76827700
C -0.19930700	4.14026900	0.74026200	C -0.35422300	4.13778100	0.55365800
C -4.82630800	-0.55998300	-1.92494900	C -4.76838900	-0.40012300	-1.74295400
C -0.87561800	4.78084100	-0.46969800	C -1.17237400	4.59409700	-0.65286300
O -3.59247200	2.41843100	-0.26251200	O -3.66301300	2.20750000	0.33994800
C -1.12383500	4.19214100	1.95685000	C -1.17928700	4.26644700	1.83453200
C -4.98059500	-0.96348900	0.54623000	C -4.95810700	-1.30146400	0.59975800
H -0.67281300	3.75738000	2.84883100	H -0.62629200	3.96891700	2.72490400

H -4.67042600	-1.56226500	1.40246900	H -4.70818200	-2.10871800	1.28972400
H -2.05278500	3.65431400	1.76286900	H -2.08151600	3.65647700	1.78163000
H -4.72293000	0.07407600	0.76099800	H -4.65566800	-0.36037700	1.06140900
H -1.37817100	5.23201900	2.18387700	H -1.48723100	5.30818700	1.96778700
H -6.07006900	-1.03064600	0.46818200	H -6.04647700	-1.28791600	0.48834100
C -2.64418400	-3.47753300	1.39982600	C -2.06172200	-3.49589400	1.44727800
C 1.64544800	2.17986300	2.95297500	C 1.62321700	2.35844100	2.87999600
H -3.73336300	-3.55314700	1.43889900	H -3.06026300	-3.40589400	1.87977800
H 1.39097800	3.16946300	3.34011600	H 1.36093400	3.35590600	3.23974200
H -2.33030000	-2.67793500	2.07333300	H -1.42464100	-2.74945600	1.92237200
H 0.82561800	1.49901700	3.18813000	H 0.81932800	1.67399900	3.15369400
H -2.24130600	-4.41847000	1.78504800	H -1.68013700	-4.48666900	1.71055300
H 2.53164900	1.83970200	3.49638700	H 2.52560300	2.05030300	3.41569200
C -2.64598000	-4.34054900	-0.97293900	C -2.95350400	-4.39253500	-0.74245900
C 3.03789100	3.23543400	1.13243600	C 2.93159400	3.40923200	0.99859700
H -2.25412100	-4.22855900	-1.98568600	H -2.98350000	-4.28418400	-1.82931000
H 3.31027100	3.23475000	0.07566300	H 3.19295000	3.37958800	-0.06044800
H -3.73695800	-4.36536000	-1.03194300	H -3.97977200	-4.36864600	-0.36865500
H 2.74894100	4.25190800	1.41228900	H 2.59262400	4.41991800	1.24048500
H -2.32422500	-5.31971300	-0.60524900	H -2.55604500	-5.38818800	-0.52472000
H 3.94148400	2.99403900	1.70055700	H 3.85156800	3.23762000	1.56574700
H 0.41638200	-0.56889800	0.42001200	H 0.44832900	-0.52385500	0.51777700
H 0.38050400	-0.15120600	-1.81622100	H 0.34223300	-0.21773500	-1.81098100
N 1.83282500	-1.33926100	-1.48147300	N 1.74730600	-1.43087900	-1.39693700
H 0.70815500	4.71117500	0.96355000	H 0.52660200	4.78451400	0.63243700
H -4.64999700	-2.45735000	-0.95922400	H -4.59812200	-2.44948800	-1.17877000
H -5.91974800	-0.58022300	-1.95844300	H -5.86126500	-0.41398200	-1.79549300
H -1.17724600	5.80187400	-0.21712700	H -1.54041100	5.60933400	-0.47687600
H -4.52830800	0.48224400	-1.80097800	H -4.47124500	0.59734800	-1.41922900
H -1.77901700	4.24105800	-0.75777600	H -2.04430700	3.95655800	-0.80882400
H -4.46757200	-0.91288800	-2.89359800	H -4.39673000	-0.56657300	-2.75593700
H -0.21626600	4.84497800	-1.33718700	H -0.58589400	4.61865400	-1.57319100
C 1.36004900	-1.77123000	-0.33347400	C 1.36050600	-1.75126500	-0.17927700
H 0.42224300	-2.30505800	-0.44483300	H 0.44089500	-2.32719200	-0.16587700
C 2.13840800	-2.28036800	0.84514900	C 2.24585300	-2.12403100	0.97722800
C 3.21324100	-3.14181800	0.60477000	C 3.31645200	-2.98880000	0.72936800
C 1.74630600	-2.05086800	2.16278100	C 1.96852700	-1.76573900	2.29466100
C 3.88558500	-3.74430800	1.65833800	C 4.09445300	-3.46903200	1.77282200
H 3.51917200	-3.33732000	-0.41651700	H 3.53569400	-3.28316100	-0.29042100
C 2.42027100	-2.65517200	3.21686700	C 2.74832100	-2.24696600	3.33929900
H 0.91403000	-1.38211400	2.34940300	H 1.14134500	-1.09537500	2.49320300
C 3.49371200	-3.50117800	2.96966300	C 3.81530500	-3.09804800	3.08300200
H 4.71823200	-4.40834500	1.45299600	H 4.92143800	-4.13795300	1.56059100
H 2.10427700	-2.46004900	4.23594700	H 2.51847300	-1.95282200	4.35762400
H 4.02161200	-3.96966700	3.79301600	H 4.42516700	-3.47140400	3.89827300
C 3.08445500	-0.75122600	-1.65171500	C 2.96648500	-0.82959000	-1.70066600
C 3.52972200	-0.63317100	-2.98039600	C 3.33852100	-0.84594200	-3.05701400
C 3.91642500	-0.23256700	-0.64443100	C 3.82786400	-0.17219700	-0.80477400
C 4.74541900	-0.04682200	-3.28823100	C 4.51210600	-0.25609800	-3.49419900
H 2.89029200	-1.02844700	-3.76206700	H 2.67711700	-1.34849000	-3.75429500
C 5.13220100	0.36015000	-0.95977800	C 5.00052600	0.42391700	-1.25036500
H 3.61837900	-0.30838700	0.39216600	H 3.58653200	-0.14108800	0.24880100
C 5.55947700	0.45723400	-2.27806500	C 5.35554800	0.38708400	-2.59287000
H 5.06122700	0.01952000	-4.32416700	H 4.77159900	-0.29595900	-4.54701200
H 5.75506900	0.74734800	-0.16001400	H 5.64684900	0.92031300	-0.53380900
H 6.51139100	0.91832300	-2.51544800	H 6.27426500	0.85163400	-2.93227700
C -2.71473900	1.68329400	-0.06457300	C -1.45248300	0.15956900	2.24188100
N -1.66765300	0.33226200	2.07804500	N -2.71434300	1.49898900	0.26296500
2Mo-cis + PhCCH-TS			2Mo-trans + PhCCH-TS		
N 1.29468200	-2.51756700	0.00000000	O 2.53894500	-3.06674700	0.00000000
O 2.09251300	-3.38731100	0.00000000	Mo 0.07125000	-1.13721300	0.00000000
P -0.00958700	-0.65227100	2.42294700	P -0.02990700	-0.63074600	2.42231600

P -0.00958700	-0.65227100	-2.42294700	P -0.02990700	-0.63074600	-2.42231600
C -1.07429300	0.88820600	2.45272700	C -1.12314800	0.89360600	2.45975800
C -1.07429300	0.88820600	-2.45272700	C -1.12314800	0.89360600	-2.45975800
H -0.38862700	1.73985100	2.44426000	H -0.45478300	1.75915400	2.46858600
H -0.38862700	1.73985100	-2.44426000	H -0.45478300	1.75915400	-2.46858600
H -1.66493600	0.95933800	3.36831000	H -1.72738900	0.94475200	3.36808300
H -1.66493600	0.95933800	-3.36831000	H -1.72738900	0.94475200	-3.36808300
C -1.97721300	0.96276900	1.23008500	C -2.01172000	0.96142900	1.22717600
C -1.97721300	0.96276900	-1.23008500	C -2.01172000	0.96142900	-1.22717600
H -2.48985500	1.93391300	1.20540200	H -2.53318100	1.92793100	1.19811400
H -2.48985500	1.93391300	-1.20540200	H -2.53318100	1.92793100	-1.19811400
H -2.74143200	0.18297100	1.25953600	H -2.76876900	0.17456600	1.24728100
H -2.74143200	0.18297100	-1.25953600	H -2.76876900	0.17456600	-1.24728100
N -1.18654000	0.77273900	0.00000000	N -1.21318900	0.77642700	0.00000000
C 1.55040900	-0.01815500	-3.26198800	C 1.48128700	0.02097700	-3.33418000
C 1.55040900	-0.01815500	3.26198800	C 1.48128700	0.02097700	3.33418000
H 1.77234000	0.85032400	-2.63166100	H 1.74027300	0.87897400	-2.70324300
H 1.77234000	0.85032400	2.63166100	H 1.74027300	0.87897400	2.70324300
C -0.81291800	-1.80877900	-3.67037300	C -0.86981900	-1.83200600	-3.59825100
C -0.81291800	-1.80877900	3.67037300	C -0.86981900	-1.83200600	3.59825100
C -2.32362100	-1.90853600	-3.47428100	C -2.36334800	-1.96030200	-3.30515100
C -2.32362100	-1.90853600	3.47428100	C -2.36334800	-1.96030200	3.30515100
C -1.45891000	-2.38677900	0.00000000	O -1.82162100	-3.47360800	0.00000000
O -2.34223800	-3.14125900	0.00000000	H -0.74851100	-1.41300900	4.60302200
H -0.62107700	-1.37673400	4.65812800	H -0.74851100	-1.41300900	-4.60302200
H -0.62107700	-1.37673400	-4.65812800	C -0.19639600	-3.20228200	3.54004100
C -0.17226700	-3.19371600	3.59460800	C -0.19639600	-3.20228200	-3.54004100
C -0.17226700	-3.19371600	-3.59460800	H 0.86368800	-3.16107900	3.79158600
H 0.89820300	-3.17348500	3.80171200	H 0.86368800	-3.16107900	-3.79158600
H 0.89820300	-3.17348500	-3.80171200	H -0.28569800	-3.63489600	2.54197400
H -0.30929300	-3.62853500	2.60211400	H -0.28569800	-3.63489600	-2.54197400
H -0.30929300	-3.62853500	-2.60211400	H -0.67980000	-3.88217900	4.24808300
H -0.63919800	-3.86151800	4.32474300	H -0.67980000	-3.88217900	-4.24808300
H -0.63919800	-3.86151800	-4.32474300	C 2.66564600	-0.94058700	-3.30241400
C 2.72458900	-0.98423900	-3.12861400	C 2.66564600	-0.94058700	3.30241400
C 2.72458900	-0.98423900	3.12861400	H 2.51937300	-1.78771300	-3.97613200
H 2.61598500	-1.85153900	-3.78358500	H 2.51937300	-1.78771300	3.97613200
H 2.61598500	-1.85153900	3.78358500	H 2.84351100	-1.33130200	-2.30033400
H 2.83241500	-1.34423700	-2.10444000	H 2.84351100	-1.33130200	2.30033400
H 2.83241500	-1.34423700	2.10444000	H 3.57091700	-0.42117600	-3.63072200
H 3.65323400	-0.48023000	-3.41296400	H 3.57091700	-0.42117600	3.63072200
H 3.65323400	-0.48023000	3.41296400	C 1.20441000	0.52070900	-4.74975700
C 1.36759400	0.45527400	-4.70108100	C 1.20441000	0.52070900	4.74975700
C 1.36759400	0.45527400	4.70108100	H 0.36939200	1.22346300	-4.79423800
H 0.53221600	1.15073900	-4.81315600	H 0.36939200	1.22346300	4.79423800
H 0.53221600	1.15073900	4.81315600	H 0.98912200	-0.30422900	-5.43350600
H 1.20459400	-0.38172500	-5.38462600	H 0.98912200	-0.30422900	5.43350600
H 1.20459400	-0.38172500	5.38462600	H 2.08692300	1.03708300	-5.13954800
H 2.27076100	0.97261000	-5.03906800	H 2.08692300	1.03708300	5.13954800
H 2.27076100	0.97261000	5.03906800	H 1.38550800	0.27193700	0.00000000
H 1.32768900	0.29456500	0.00000000	H -0.47852000	1.49224400	0.00000000
H -0.44436300	1.48098500	0.00000000	C 2.09295300	1.68380300	0.00000000
C 2.05939100	1.72250500	0.00000000	H -2.80912100	-2.67857000	-3.99967200
H -2.74227700	-2.59358000	-4.21761500	H -2.53995300	-2.33119300	-2.29405700
H -2.57300800	-2.30483500	-2.48887800	H -2.89872000	-1.01687700	-3.42991600
H -2.82932000	-0.94896400	-3.60023700	H -2.80912100	-2.67857000	3.99967200
H -2.74227700	-2.59358000	4.21761500	H -2.89872000	-1.01687700	3.42991600
H -2.82932000	-0.94896400	3.60023700	H -2.53995300	-2.33119300	2.29405700
H -2.57300800	-2.30483500	2.48887800	C 1.48020300	2.76117400	0.00000000
C 1.44057900	2.79465000	0.00000000	C 1.61519200	-2.36714600	0.00000000
C 0.63799200	3.95051900	0.00000000	N -1.11747600	-2.51854200	0.00000000
C 0.23322000	4.56006100	1.20713400	C 0.66630500	3.90749900	0.00000000
C 0.23322000	4.56006100	-1.20713400	C 0.25561600	4.51438500	1.20732800

C -0.54972000	5.70149800	1.19913300	C 0.25561600	4.51438500	-1.20732800
H 0.55797800	4.13118000	2.14808500	C -0.53815600	5.64815500	1.19904500
C -0.54972000	5.70149800	-1.19913300	H 0.58594700	4.08994800	2.14836500
H 0.55797800	4.13118000	-2.14808500	C -0.53815600	5.64815500	-1.19904500
C -0.95373100	6.28071200	0.00000000	H 0.58594700	4.08994800	-2.14836500
H -0.84316500	6.15007900	2.14240800	C -0.94809700	6.22368000	0.00000000
H -0.84316500	6.15007900	-2.14240800	H -0.83530500	6.09419400	2.14240300
H -1.56454500	7.17578800	0.00000000	H -0.83530500	6.09419400	-2.14240300
H 3.03349900	1.27396300	0.00000000	H -1.56717700	7.11302700	0.00000000
Mo 0.10104300	-1.15448400	0.00000000	H 3.07333600	1.24700900	0.00000000
2Mo-cis + PhCCH-TS-H_M transfer to Ph-C			2Mo-trans + PhCCH-TS-H_M transfer to Ph-C		
C -2.71791600	-0.63330200	0.00000000	O 0.23110400	-3.24569200	0.00000000
O -3.86032900	-0.84439200	0.00000000	P -0.65902900	0.20036700	2.42840500
Mo -0.75803000	-0.30236000	0.00000000	P -0.65902900	0.20036700	-2.42840500
P -0.65118000	0.18302900	2.43118900	C -0.83942500	2.06419400	2.45244300
P -0.65118000	0.18302900	-2.43118900	C -0.83942500	2.06419400	-2.45244300
C -0.84129800	2.04297700	2.44652100	H 0.17702700	2.46822600	2.42685000
C -0.84129800	2.04297700	-2.44652100	H 0.17702700	2.46822600	-2.42685000
H 0.17429900	2.44783500	2.40648400	H -1.31364200	2.42498500	3.36761400
H 0.17429900	2.44783500	-2.40648400	H -1.31364200	2.42498500	-3.36761400
H -1.30301500	2.40535800	3.36700100	C -1.59447800	2.55268600	1.22505800
H -1.30301500	2.40535800	-3.36700100	C -1.59447800	2.55268600	-1.22505800
C -1.61188100	2.52940600	1.22784300	H -1.56574300	3.65159800	1.18770300
C -1.61188100	2.52940600	-1.22784300	H -1.56574300	3.65159800	-1.18770300
H -1.59631400	3.62857800	1.19539300	H -2.64445500	2.25345300	1.26159000
H -1.59631400	3.62857800	-1.19539300	H -2.64445500	2.25345300	-1.26159000
H -2.65786200	2.21741400	1.26972000	N -0.99938600	1.98886300	0.00000000
H -2.65786200	2.21741400	-1.26972000	C 0.95828300	-0.00676600	-3.36338300
N -1.01192700	1.97885700	0.00000000	C 0.95828300	-0.00676600	3.36338300
C 0.98700200	-0.02148300	-3.32912300	H 1.65487700	0.49536000	-2.68297900
C 0.98700200	-0.02148300	3.32912300	H 1.65487700	0.49536000	2.68297900
H 1.66905600	0.47103100	-2.62778500	C -1.99903000	-0.43300400	-3.58599000
H 1.66905600	0.47103100	2.62778500	C -1.99903000	-0.43300400	3.58599000
C -1.94159000	-0.47441300	-3.63515600	C -3.33883800	0.26113900	-3.34906100
C -1.94159000	-0.47441300	3.63515600	C -3.33883800	0.26113900	3.34906100
C -3.28027600	0.24956500	-3.51332600	O -3.66323000	-1.21215500	0.00000000
C -3.28027600	0.24956500	3.51332600	H -1.66076200	-0.19720300	4.60102300
N -0.34682400	-2.06766500	0.00000000	H -1.66076200	-0.19720300	-4.60102300
O -0.05287500	-3.21270400	0.00000000	C -2.15816400	-1.94713500	3.45024300
C -2.13279500	-1.97726100	3.43122200	C -2.15816400	-1.94713500	-3.45024300
C -2.13279500	-1.97726100	-3.43122200	H -1.22994500	-2.48755200	3.63538800
H -1.20604400	-2.53995700	3.54463800	H -1.22994500	-2.48755200	-3.63538800
H -1.20604400	-2.53995700	-3.54463800	H -2.50157500	-2.21074200	2.44865900
H -2.52150600	-2.18319000	2.43217000	H -2.50157500	-2.21074200	-2.44865900
H -2.52150600	-2.18319000	-2.43217000	H -2.90215300	-2.30558900	4.16831200
H -2.85044400	-2.36346100	4.16150700	H -2.90215300	-2.30558900	-4.16831200
H -2.85044400	-2.36346100	-4.16150700	C 1.39226100	-1.46550200	-3.48067500
C 1.40774000	-1.48519200	-3.43839100	C 1.39226100	-1.46550200	3.48067500
C 1.40774000	-1.48519200	3.43839100	H 0.81323000	-1.99529100	-4.24093300
H 0.83637900	-2.00893300	-4.20886000	H 0.81323000	-1.99529100	4.24093300
H 0.83637900	-2.00893300	4.20886000	H 1.28765000	-2.00070800	-2.53641900
H 1.28029400	-2.01914300	-2.49552500	H 1.28765000	-2.00070800	2.53641900
H 1.28029400	-2.01914300	2.49552500	H 2.44268300	-1.51541800	-3.78065800
H 2.46282200	-1.54761200	-3.71911100	H 2.44268300	-1.51541800	3.78065800
H 2.46282200	-1.54761200	3.71911100	C 1.00775200	0.69347600	-4.71912300
C 1.07927300	0.68271800	-4.68026100	C 1.00775200	0.69347600	4.71912300
C 1.07927300	0.68271800	4.68026100	H 0.74734000	1.75182600	-4.65777600
H 0.82649200	1.74327000	-4.62134400	H 0.74734000	1.75182600	4.65777600
H 0.82649200	1.74327000	4.62134400	H 0.33953900	0.22091900	-5.44379100
H 0.42746000	0.21977000	-5.42580600	H 0.33953900	0.22091900	5.44379100
H 0.42746000	0.21977000	5.42580600	H 2.02029600	0.63022700	-5.12916800
H 2.10219000	0.61262100	-5.06275300	H 2.02029600	0.63022700	5.12916800

H	2.10219000	0.61262100	5.06275300	H	1.02767400	0.34902500	0.00000000
H	0.99268300	0.41703100	0.00000000	H	0.00832200	2.26968800	0.00000000
H	-0.01019000	2.27165000	0.00000000	C	2.26268200	1.49699600	0.00000000
C	2.25065800	1.54576100	0.00000000	C	3.39622000	0.58094800	0.00000000
C	3.36400200	0.60595400	0.00000000	C	3.29161800	-0.80761300	0.00000000
C	3.22633900	-0.78034400	0.00000000	C	4.42791400	-1.60593100	0.00000000
C	4.34489800	-1.60335400	0.00000000	C	5.69069200	-1.02965700	0.00000000
C	5.62049500	-1.05570200	0.00000000	C	4.67798000	1.15507600	0.00000000
C	4.65800900	1.15134100	0.00000000	C	5.80957000	0.35719800	0.00000000
C	5.77131300	0.32799100	0.00000000	H	2.30259700	-1.24694300	0.00000000
H	2.22551300	-1.19549400	0.00000000	H	4.32099100	-2.68507100	0.00000000
H	4.21406200	-2.67986400	0.00000000	H	6.57753700	-1.65374800	0.00000000
H	6.49290400	-1.69988200	0.00000000	H	4.76665500	2.23527100	0.00000000
H	4.77068600	2.22931700	0.00000000	H	6.79086100	0.81939000	0.00000000
H	6.76292100	0.76757900	0.00000000	H	-4.08589400	-0.14758400	-4.03606400
H	-1.54250900	-0.29753800	4.63970400	H	-3.70171000	0.08746100	-2.33425700
H	-1.54250900	-0.29753800	-4.63970400	H	-3.29309000	1.33758900	-3.52523000
H	-3.99434800	-0.18331700	-4.22033300	H	-4.08589400	-0.14758400	4.03606400
H	-3.99434800	-0.18331700	4.22033300	H	-3.29309000	1.33758900	3.52523000
H	-3.70480800	0.13479400	-2.51421000	H	-3.70171000	0.08746100	2.33425700
H	-3.70480800	0.13479400	2.51421000	C	1.88807600	2.67807300	0.00000000
H	-3.20720700	1.31505700	-3.73996500	H	1.97615700	3.74234200	0.00000000
H	-3.20720700	1.31505700	3.73996500	C	-0.15505600	-2.15254700	0.00000000
C	1.88764700	2.72843300	0.00000000	N	-2.54064600	-0.82823200	0.00000000
H	1.92431900	3.79470700	0.00000000	Mo	-0.80496600	-0.28309500	0.00000000
2Mo-cis + PhCCH-interm				2Mo-trans + PhCCH-interm			
O	-3.74329800	-1.02435300	0.00000000	N	-2.47983000	-0.84948100	0.00000000
Mo	-0.71943600	-0.28790300	0.00000000	O	-3.60097800	-1.23179300	0.00000000
P	-0.64678600	0.20425400	2.44813200	Mo	-0.77888400	-0.27740200	0.00000000
P	-0.64678600	0.20425400	-2.44813200	P	-0.64447900	0.21553500	2.44295700
C	-0.92548000	2.05134000	2.44798000	P	-0.64447900	0.21553500	-2.44295700
C	-0.92548000	2.05134000	-2.44798000	C	-0.91908700	2.06659900	2.45147500
H	0.06958600	2.50465800	2.40291000	C	-0.91908700	2.06659900	-2.45147500
H	0.06958600	2.50465800	-2.40291000	H	0.07560900	2.52148000	2.41274400
H	-1.40087800	2.39780000	3.36733000	H	0.07560900	2.52148000	-2.41274400
H	-1.40087800	2.39780000	-3.36733000	H	-1.39969300	2.41114900	3.36915200
C	-1.72444900	2.48834100	1.23004400	H	-1.39969300	2.41114900	-3.36915200
C	-1.72444900	2.48834100	-1.23004400	C	-1.71353200	2.50499800	1.23032300
H	-1.77580000	3.58528800	1.19377800	C	-1.71353200	2.50499800	-1.23032300
H	-1.77580000	3.58528800	-1.19377800	H	-1.75803800	3.60232200	1.19163900
H	-2.74820200	2.11085800	1.26897900	H	-1.75803800	3.60232200	-1.19163900
H	-2.74820200	2.11085800	-1.26897900	H	-2.73970800	2.13399900	1.26947000
N	-1.08980100	1.97395800	0.00000000	H	-2.73970800	2.13399900	-1.26947000
C	0.99628000	0.07555300	-3.34844900	N	-1.08634000	1.98158400	0.00000000
C	0.99628000	0.07555300	3.34844900	C	0.98786000	0.08249800	-3.36153000
H	1.66662000	0.58431500	-2.64689400	C	0.98786000	0.08249800	3.36153000
H	1.66662000	0.58431500	2.64689400	H	1.66565300	0.59655300	-2.67082000
C	-1.91567800	-0.52150800	-3.63138500	H	1.66565300	0.59655300	2.67082000
C	-1.91567800	-0.52150800	3.63138500	C	-1.94692500	-0.49593500	-3.59560600
C	-3.28441700	0.14428300	-3.51199000	C	-1.94692500	-0.49593500	3.59560600
C	-3.28441700	0.14428300	3.51199000	C	-3.31689000	0.14950000	-3.39692300
O	0.00688500	-3.19073800	0.00000000	C	-3.31689000	0.14950000	3.39692300
H	-1.52616000	-0.33381400	4.63763000	C	-0.13703600	-2.15675100	0.00000000
H	-1.52616000	-0.33381400	-4.63763000	O	0.19837500	-3.26324500	0.00000000
C	-2.03727600	-2.03037300	3.41868500	H	-1.60054600	-0.26908100	4.60977600
C	-2.03727600	-2.03037300	-3.41868500	H	-1.60054600	-0.26908100	-4.60977600
H	-1.08275800	-2.54832900	3.51195300	C	-2.04539400	-2.01227100	3.42992100
H	-1.08275800	-2.54832900	-3.51195300	C	-2.04539400	-2.01227100	-3.42992100
H	-2.43663300	-2.25026200	2.42708000	H	-1.08958700	-2.51585300	3.57317600
H	-2.43663300	-2.25026200	-2.42708000	H	-1.08958700	-2.51585300	-3.57317600
H	-2.72162300	-2.45425900	4.15960000	H	-2.41111100	-2.27052500	2.43488900
H	-2.72162300	-2.45425900	-4.15960000	H	-2.41111100	-2.27052500	-2.43488900

C	1.46955800	-1.36936000	-3.48841800	H	-2.74942500	-2.41680600	4.16327000
C	1.46955800	-1.36936000	3.48841800	H	-2.74942500	-2.41680600	-4.16327000
H	0.90944500	-1.90143900	-4.26150500	C	1.46732200	-1.35962100	-3.50561900
H	0.90944500	-1.90143900	4.26150500	C	1.46732200	-1.35962100	3.50561900
H	1.37950400	-1.92474700	-2.55374400	H	0.90599400	-1.89353400	-4.27636300
H	1.37950400	-1.92474700	2.55374400	H	0.90599400	-1.89353400	4.27636300
H	2.52260700	-1.38363300	-3.78098400	H	1.38470400	-1.91634900	-2.57145300
H	2.52260700	-1.38363300	3.78098400	H	1.38470400	-1.91634900	2.57145300
C	1.04728600	0.80660400	-4.68770000	H	2.51877800	-1.36736300	-3.80401800
C	1.04728600	0.80660400	4.68770000	H	2.51877800	-1.36736300	3.80401800
H	0.76674700	1.85830000	-4.60600100	C	1.01646900	0.81086000	-4.70314900
H	0.76674700	1.85830000	4.60600100	C	1.01646900	0.81086000	4.70314900
H	0.40064100	0.33755300	-5.43406200	H	0.73312000	1.86155200	-4.62018000
H	0.40064100	0.33755300	5.43406200	H	0.73312000	1.86155200	4.62018000
H	2.06738600	0.77356400	-5.08120800	H	0.36046500	0.33680600	-5.43805200
H	2.06738600	0.77356400	5.08120800	H	0.36046500	0.33680600	5.43805200
H	1.12339200	0.72095500	0.00000000	H	2.03072800	0.78039100	-5.11147300
H	-0.11980500	2.33647700	0.00000000	H	2.03072800	0.78039100	5.11147300
C	2.08746100	1.44059300	0.00000000	H	1.15045400	0.67789200	0.00000000
C	3.28331700	0.57159000	0.00000000	H	-0.11095000	2.32586800	0.00000000
C	3.18298600	-0.81866500	0.00000000	C	2.10686300	1.41662000	0.00000000
C	4.31615300	-1.62387200	0.00000000	C	3.31333600	0.56097700	0.00000000
C	5.57898900	-1.04854200	0.00000000	C	3.23341300	-0.82995200	0.00000000
C	4.56445800	1.14058900	0.00000000	C	4.37683300	-1.62040900	0.00000000
C	5.69395000	0.34046800	0.00000000	C	5.63167800	-1.02806200	0.00000000
H	2.19618600	-1.27140200	0.00000000	C	4.58694700	1.14704900	0.00000000
H	4.20787800	-2.70333800	0.00000000	C	5.72719900	0.36244600	0.00000000
H	6.46621500	-1.67243800	0.00000000	H	2.25360500	-1.29592500	0.00000000
H	4.63400300	2.22265200	0.00000000	H	4.28280200	-2.70121600	0.00000000
H	6.67635700	0.80153900	0.00000000	H	6.52735500	-1.63972600	0.00000000
H	-3.97751800	-0.32210000	-4.21821700	H	4.64124900	2.22996600	0.00000000
H	-3.70586300	0.01416400	-2.51336700	H	6.70310800	0.83712300	0.00000000
H	-3.25785800	1.21085700	-3.74298200	H	-4.03250300	-0.30088800	-4.09098200
H	-3.97751800	-0.32210000	4.21821700	H	-3.69542400	-0.02058700	-2.38715500
H	-3.25785800	1.21085700	3.74298200	H	-3.31065700	1.22336900	-3.59271200
H	-3.70586300	0.01416400	2.51336700	H	-4.03250300	-0.30088800	4.09098200
C	2.05708400	2.74722600	0.00000000	H	-3.31065700	1.22336900	3.59271200
H	1.19417700	3.41516500	0.00000000	H	-3.69542400	-0.02058700	2.38715500
N	-0.27451900	-2.04805800	0.00000000	C	2.06863400	2.72284600	0.00000000
C	-2.61862300	-0.73305100	0.00000000	H	1.20209300	3.38504500	0.00000000
2Mo-cis + PhCCH-TS-H_N transfer to C-H				2Mo-trans + PhCCH-TS-H_N transfer to C-H			
Mo	0.00016900	-0.72938100	-0.29061800	N	0.00277600	-2.50396600	-0.82715800
N	0.00013600	-0.98976600	1.97547900	O	0.00415300	-3.62998400	-1.19926800
H	-0.00003000	1.10577900	0.60979300	Mo	0.00090400	-0.78603300	-0.27870600
H	-0.00032400	0.00988600	2.30561200	P	2.43771300	-0.64062400	0.20278100
C	-0.00026500	2.07780700	1.43272300	P	-2.43632800	-0.64581800	0.20241200
C	-0.00056000	3.28531700	0.57529400	C	2.45479600	-0.82389100	2.06499800
C	-0.00047000	3.19959900	-0.81431500	C	-2.45345500	-0.82971100	2.06456800
C	-0.00073600	4.34485800	-1.60139200	H	2.42678600	0.19256600	2.46914200
C	-0.00110100	5.59907600	-1.00630400	H	-2.42801700	0.18668400	2.46903400
C	-0.00119300	5.69702400	0.38345800	H	3.36928400	-1.29704200	2.42855100
C	-0.00092500	4.55454500	1.16590500	H	-3.36689000	-1.30518600	2.42773200
P	2.44248700	-0.64254300	0.18940800	C	1.22651800	-1.58007900	2.54878400
P	-2.44218600	-0.64338200	0.18935900	C	-1.22347700	-1.58309500	2.54842000
N	0.00004800	-0.30233000	-2.05567700	H	1.18606200	-1.55130100	3.64744300
C	0.00039800	-2.65298900	-0.67142800	H	-1.18330300	-1.55448100	3.64709400
C	-3.35356800	0.98754500	-0.01485600	H	1.26287800	-2.62988800	2.24985400
C	3.35315300	0.98870500	-0.01541000	H	-1.25729200	-2.63291300	2.24922400
C	-3.62523400	-1.94655300	-0.47678200	N	0.00086800	-0.98198500	1.98455700
C	3.62609900	-1.94564000	-0.47583900	C	-3.37715200	0.96792900	-0.00546100
O	0.00051900	-3.78613700	-0.92965400	C	3.37490500	0.97518800	-0.00543700
C	2.45026500	-0.83384800	2.04731900	H	-2.70111200	1.67203300	0.49225200

C -2.45005000	-0.83544400	2.04720300	H 2.69693600	1.67798600	0.49150300
H 2.41287200	0.18239800	2.45112900	C -3.58061500	-1.99135700	-0.44114700
H -2.41332700	0.18066900	2.45141200	C 3.58525100	-1.98378700	-0.43997600
H 3.36717200	-1.29975600	2.41320700	C -3.34849500	-3.32963400	0.25744400
H -3.36671100	-1.30203700	2.41281800	C 3.35584500	-3.32239200	0.25888500
C 1.22594200	-1.59758600	2.52846500	C 0.00029500	-0.14496400	-2.15559800
C -1.22529900	-1.59859000	2.52819200	O -0.00006600	0.20571500	-3.25939100
H 1.18874400	-1.57869000	3.62729200	H 4.60164100	-1.64383500	-0.21304900
H -1.18819700	-1.58002100	3.62702700	H -4.59785500	-1.65374500	-0.21455600
H 1.26271600	-2.64442500	2.21971800	C 3.43781000	-2.14397700	-1.95287100
H -1.26139000	-2.64535200	2.21910000	C -3.43214300	-2.15073800	-1.95402400
H -2.66168300	1.68015000	0.47671700	H 3.61196000	-1.21466700	-2.49490500
H 2.66108400	1.68106100	0.47626000	H -3.60869200	-1.22176200	-2.49586000
C -3.49242700	-3.28466800	0.24630900	H 2.43721900	-2.49555100	-2.20909800
C 3.49278200	-3.28371400	0.24723500	H -2.43045100	-2.49939400	-2.20994500
O -0.00007000	-0.01709200	-3.20062200	H 4.15855400	-2.88268400	-2.31650900
H 4.63439900	-1.55604800	-0.29942800	H -4.15067000	-2.89135700	-2.31815300
H -4.63368200	-1.55700000	-0.30114800	C -3.50512500	1.39616500	-1.46500500
C 3.41951600	-2.13098400	-1.97904500	C 3.50265300	1.40288700	-1.46516000
C -3.41753800	-2.13180500	-1.97984900	H -4.26301500	0.80934000	-1.98958500
H 3.53293500	-1.20235300	-2.53847000	H 4.26242200	0.81774900	-1.98890700
H -3.52989700	-1.20301800	-2.53923500	H -2.56263100	1.30058800	-2.00513400
H 2.42125700	-2.52040100	-2.18648100	H 2.56074900	1.30446200	-2.00580700
H -2.41936300	-2.52182200	-2.18652900	H -3.81373200	2.44382200	-1.51500700
H 4.14967400	-2.84710300	-2.36799800	H 3.80851000	2.45132700	-1.51561700
H -4.14783800	-2.84740200	-2.36949600	C -4.72940400	1.00954400	0.70230300
C -3.47351000	1.40701900	-1.47806000	C 4.72668200	1.02043500	0.70300900
C 3.47244600	1.40807100	-1.47869900	H -4.65984400	0.75643500	1.76179600
H -4.23769400	0.82557700	-1.99983900	H 4.65717700	0.76779100	1.76261500
H 4.23699000	0.82718300	-2.00056200	H -5.45182400	0.33356800	0.23738600
H -2.53078900	1.29566200	-2.01576800	H 5.45094700	0.34591100	0.23886100
H 2.52970300	1.29586800	-2.01618900	H -5.14632300	2.01884300	0.63587400
H -3.76855200	2.45810300	-2.53733400	H 5.14123100	2.03068500	0.63620000
H 3.76662500	2.45938500	-1.53817800	H -0.00060000	1.12978000	0.55333800
C -4.70307500	1.06247900	0.69486500	H -0.00040400	0.02300400	2.29018900
C 4.70282100	1.06439800	0.69392300	C -0.00246000	2.10496400	1.40650200
H -4.63635100	0.81321000	1.75562900	C -0.00374500	3.31991600	0.55957400
H 4.63656600	0.81497700	1.75468300	C -0.00278200	3.25460100	-0.83044500
H -5.44218400	0.40071100	0.23573500	C -0.00398900	4.41002200	-1.60248800
H 5.44218900	0.40313000	0.23449300	C -0.00619300	5.65605700	-0.99079500
H -5.09765800	2.08053700	0.62457500	C -0.00596100	4.58169200	1.16689000
H 5.09676300	2.08270500	0.62362400	C -0.00717500	5.73466700	0.40018400
H -0.00017000	2.21611000	-1.27428500	H -0.00106200	2.27875300	-1.30365900
H -0.00065700	4.25409000	-2.68232500	H -0.00320300	4.33332400	-2.68451400
H -0.00131200	6.49506100	-1.61754400	H -0.00714500	6.56024700	-1.58978500
H -0.00098900	4.61313500	2.24892100	H -0.00668200	4.62569800	2.25052600
H -0.00147600	6.67295400	0.85765900	H -0.00889800	6.70387800	0.88795300
H 4.19380200	-4.00290600	-0.18663500	H -4.03296100	-4.07691600	-0.15484000
H -4.19295800	-4.00391300	-0.18825800	H -2.33291900	-3.69401400	0.09162300
H 3.72062000	-3.21305900	1.31253900	H -3.53244500	-3.28181300	1.33241200
H -3.72123000	-3.21413200	1.31141300	H 4.04207300	-4.06828000	-0.15299300
H 2.49039000	-3.70043300	0.13247000	H 3.53934500	-3.27390400	1.33390000
H -2.48988100	-3.70126300	0.13241000	H 2.34111900	-3.68903300	0.09282200
C -0.00023900	1.91998400	2.69480200	C -0.00277800	1.93642600	2.66480600
H -0.00005000	1.55852800	3.69722100	H -0.00268900	1.57787900	3.66805400
2Mo-cis + PhCHCH₂-TS-H_M transfer			2Mo-trans + PhCHCH₂-TS-H_M transfer		
O -2.33315200	2.47269600	-1.90714600	O -2.45743900	2.69835400	-1.33305900
P 1.28857300	1.90284400	-0.02704800	P 1.32483900	1.87774200	-0.05562200
P -2.44053800	-1.23414700	-0.07413500	P -2.44531600	-1.21210700	-0.09546200
C 2.23568900	0.83652400	-1.23582000	C 2.25396800	0.81170300	-1.28354700
C -1.57333600	-2.30476200	-1.34195600	C -1.61158800	-2.28378400	-1.38978600
H 2.83665400	0.13954400	-0.64538400	H 2.86588800	0.11384400	-0.70494600

H	-1.01261500	-3.05839300	-0.78246900	H	-1.07222700	-3.06781700	-0.85124700
H	2.92964600	1.42407400	-1.84076100	H	2.93608000	1.40038000	-1.90139400
H	-2.28116500	-2.83891900	-1.97924900	H	-2.33651100	-2.78061900	-2.03852300
C	1.29309100	0.05077300	-2.13532700	C	1.29508900	0.02878300	-2.16694700
C	-0.60894300	-1.48924800	-2.19106400	C	-0.62813200	-1.47497700	-2.22244700
H	1.87051700	-0.65985400	-2.74143300	H	1.85972800	-0.69352500	-2.77156100
H	-0.01146900	-2.16159100	-2.82236300	H	-0.03970300	-2.15011500	-2.85941600
H	0.76214000	0.71634600	-2.81979100	H	0.76650700	0.69411300	-2.85318200
H	-1.15235000	-0.81212200	-2.85376600	H	-1.15629000	-0.78074100	-2.87965800
N	0.27713600	-0.67036300	-1.34098100	N	0.27029200	-0.67420700	-1.36571800
C	-2.64990600	-2.46252300	1.33922500	C	-2.71836400	-2.48739900	1.26462400
C	2.46207200	1.92415400	1.44337700	C	2.56382400	1.93411900	1.35990100
H	-1.62641400	-2.84034000	1.43398000	H	-1.70410700	-2.88406800	1.38332700
H	2.60873800	0.84970800	1.59139000	H	2.69851000	0.86421600	1.54837000
C	-4.17705100	-0.99608900	-0.75932300	C	-4.14805300	-0.87226500	-0.81405500
C	1.38239900	3.63913700	-0.74665900	C	1.35363500	3.59517600	-0.81855500
C	-4.17722400	-0.60933200	-2.23614600	C	-4.07018700	-0.36975200	-2.25415100
C	1.06602600	3.67202600	-2.24003400	C	0.91807300	3.57877900	-2.28239100
O	-2.11084900	2.10143100	2.47606700	O	-1.81623300	1.82691300	2.88567700
H	2.41880300	3.96526300	-0.61185700	H	2.39754000	3.92370600	-0.77574500
H	-4.67575300	-1.96563100	-0.66166300	H	-4.67108200	-1.83433000	-0.81464700
C	0.45808500	4.58406200	0.01941200	C	0.49092100	4.56527400	-0.01280000
C	-4.93352300	0.04056200	0.06952900	C	-4.91852300	0.11551700	0.06033500
H	0.70782500	4.64720600	1.07907500	H	0.81213900	4.64921800	1.02563200
H	-5.02446100	-0.24640400	1.11794100	H	-5.05467000	-0.24551700	1.08034600
H	-0.58094300	4.25728200	-0.05699800	H	-0.55434700	4.25254100	-0.01559000
H	-4.42917600	1.00844100	0.03361900	H	-4.40243500	1.07573000	0.11121900
H	0.52697000	5.59298000	-0.39821600	H	0.54490900	5.56345400	-0.45781400
H	-5.94469400	0.17039500	-0.32746000	H	-5.91173800	0.28824800	-0.36480600
C	-3.00774600	-1.78119400	2.65750200	C	-3.12488300	-1.86663800	2.59799300
C	1.81269800	2.47354100	2.71065000	C	2.00234400	2.55662300	2.63474100
H	-4.04217400	-1.43114800	2.66645800	H	-4.15709400	-1.51090600	2.58237400
H	1.68895500	3.55774100	2.66786900	H	1.91825600	3.64230800	2.55329500
H	-2.36151800	-0.92430500	2.85409900	H	-2.48485700	-1.02529700	2.86502800
H	0.83292700	2.02721800	2.88556700	H	1.01822000	2.15835600	2.88191300
H	-2.89982600	-2.48925000	3.48468800	H	-3.05424300	-2.61579000	3.39226800
H	2.44622300	2.25649500	3.57603900	H	2.67399300	2.34918600	3.47324800
C	-3.56469500	-3.64826700	1.04550700	C	-3.63510400	-3.64591400	0.87949600
C	3.82334900	2.56072800	1.17924400	C	3.92169700	2.52787400	0.99430200
H	-3.32536000	-4.14062800	0.09974300	H	-3.35636400	-4.10650000	-0.07112900
H	4.30209600	2.16916000	0.27882200	H	4.34970200	2.07753000	0.09632900
H	-4.61535500	-3.34990000	1.01578900	H	-4.67780900	-3.32719200	0.80934800
H	3.74942700	3.64655700	1.08179800	H	3.86042500	3.60780600	0.83916800
H	-3.46736800	-4.39688100	1.83764400	H	-3.58934900	-4.42525400	1.64610500
H	4.49505900	2.36127600	2.01982000	H	4.62992500	2.36269600	1.81190700
H	0.22271400	-0.56488100	1.23270600	H	0.21170900	-0.55494300	1.28961400
H	0.77474000	-1.31553700	-0.70803500	H	0.75888800	-1.33036400	-0.73601400
C	1.00837100	-1.77614200	1.80598500	C	0.94365200	-1.77150600	1.82352200
H	-5.20992600	-0.49915600	-2.58044900	H	-5.08219900	-0.18886200	-2.62846000
H	-3.67550000	0.34414300	-2.40342200	H	-3.52408600	0.57190500	-2.32101400
H	-3.70696100	-1.36471400	-2.86913000	H	-3.60384000	-1.09333900	-2.92592600
H	1.14240200	4.70127400	-2.60335500	H	0.94152000	4.59848200	-2.67823400
H	1.76040500	3.07065300	-2.83017700	H	1.57800200	2.97516900	-2.90863900
H	0.05032200	3.33099400	-2.44390100	H	-0.10308600	3.21047900	-2.39195800
H	0.13960100	-2.08285500	2.37421500	H	0.07036200	-2.07487400	2.38826300
C	1.54591300	-2.66415200	0.88899500	C	1.47000800	-2.66591400	0.90111400
H	0.91266300	-3.47471500	0.53579100	H	0.82189200	-3.45933200	0.53640400
N	-1.61895400	1.54375900	1.56066200	Mo	-0.82850400	0.66155000	0.15128600
Mo	-0.84728700	0.65578600	0.18139600	C	-1.45813600	1.40773200	1.86695700
C	-1.77166500	1.77519000	-1.16657700	N	-1.80296500	1.86328700	-0.80111700
H	1.66757300	-1.12680200	2.37265600	H	1.61855700	-1.15553900	2.41000400
C	2.89328300	-2.66600700	0.36275100	C	2.81850800	-2.68845600	0.38350800
C	3.24102600	-3.56131100	-0.67017600	C	3.15938500	-3.58712600	-0.64999400

C 3.92432400 -1.83424600 0.84451700	C 3.86035800 -1.87291200 0.87163700
C 4.52158500 -3.61261000 -1.19377100	C 4.44187500 -3.65714700 -1.16594400
H 2.47911000 -4.23242900 -1.05627400	H 2.38980600 -4.24627500 -1.04160100
C 5.20455400 -1.88516700 0.31577700	C 5.14275100 -1.94327000 0.35046000
H 3.72676600 -1.15956800 1.67000500	H 3.66896700 -1.19696200 1.69752500
C 5.51825400 -2.76874900 -0.71211400	C 5.44915500 -2.82969100 -0.67720300
H 4.74668700 -4.31933700 -1.98604400	H 4.66051300 -4.36598800 -1.95818900
H 5.97287600 -1.23448600 0.72115500	H 5.91859600 -1.30514300 0.76154400
H 6.52166700 -2.80857600 -1.11970000	H 6.45416300 -2.88439300 -1.07901900
2Mo-cis + PhCHCH₂-interm	2Mo-trans + PhCHCH₂-interm
O -2.36743800 2.47344200 -1.77531900	O -2.45281000 2.63505700 -1.35865600
P 1.28506200 1.89586300 -0.04673500	P 1.31608900 1.87600700 -0.06115400
P -2.48335900 -1.24585600 -0.06432600	P -2.47328900 -1.23269300 -0.08070200
C 2.22852200 0.79542200 -1.21890400	C 2.25299500 0.77527000 -1.24397300
C -1.60194900 -2.33660700 -1.29684400	C -1.62192200 -2.31851700 -1.34497600
H 2.82352600 0.11179300 -0.60626500	H 2.85405300 0.08993700 -0.63883200
H -1.05729800 -3.08300400 -0.71330500	H -1.09394600 -3.09563200 -0.78662000
H 2.92815200 1.36107000 -1.83759800	H 2.94617800 1.34374200 -1.86807000
H -2.29958900 -2.87565000 -1.94107900	H -2.33703900 -2.82075200 -2.00027800
C 1.28303300 -0.01320600 -2.09251100	C 1.30109800 -0.02954300 -2.11396600
C -0.61206400 -1.53919600 -2.13267100	C -0.61886700 -1.52290700 -2.16676700
H 1.86034500 -0.75316100 -2.66149500	H 1.87232600 -0.77636200 -2.68029000
H 0.00470000 -2.22956000 -2.72407200	H -0.01237900 -2.21245300 -2.76968600
H 0.76604800 0.62795600 -2.81057500	H 0.78995800 0.61326000 -2.83441400
H -1.13344400 -0.88259700 -2.83289200	H -1.13006100 -0.84736700 -2.85638300
N 0.25872000 -0.70470900 -1.27624800	N 0.26278400 -0.70657400 -1.30329500
C -2.74251100 -2.45083300 1.35908500	C -2.77128100 -2.48176600 1.29745800
C 2.45316800 1.98053900 1.42358500	C 2.52888600 1.98964600 1.37169400
H -1.71538100 -2.79072300 1.52969800	H -1.75674200 -2.86401800 1.45490300
H 2.51338200 0.92205600 1.69594900	H 2.60563200 0.93564700 1.65745900
C -4.19726000 -0.96217800 -0.78385300	C -4.16190600 -0.87880600 -0.82239600
C 1.33106100 3.61373100 -0.81060400	C 1.31980500 3.57245100 -0.86839200
C -4.15837500 -0.62322000 -2.27228800	C -4.06443300 -0.41492100 -2.27442600
C 1.06769400 3.59299400 -2.31471300	C 0.93591900 3.50658900 -2.34536200
O -2.04607600 2.03667600 2.55448500	O -1.83325600 1.85077900 2.88137400
H 2.35007200 3.97996900 -0.64736900	H 2.35397100 3.92657100 -0.79872600
H -4.72959100 -1.91136000 -0.66486000	H -4.69741300 -1.83377700 -0.80386600
C 0.34836500 4.54946800 -0.10748700	C 0.40880300 4.54551900 -0.12081100
C -4.93492900 0.12341200 -0.00160300	C -4.92830100 0.13904900 0.02056100
H 0.52225500 4.61468500 0.96654800	H 0.66897900 4.64185700 0.93304400
H -5.03061300 -0.11371500 1.05841100	H -5.06807200 -0.18976600 1.05069200
H -0.68032100 4.21771500 -0.25672300	H -0.63355400 4.23023700 -0.18061300
H -4.41712400 1.08093500 -0.08135300	H -4.40923600 1.09848800 0.04308800
H 0.43894200 5.55827300 -0.52118000	H 0.48452700 5.53886700 -0.57332800
H -5.94348200 0.25111500 -0.40563000	H -5.91968500 0.30307100 -0.41197500
C -3.21633900 -1.76694500 2.63902800	C -3.22830300 -1.84372900 2.60619200
C 1.86067000 2.72969900 2.61466000	C 1.98282000 2.75526100 2.57397900
H -4.26572800 -1.47122200 2.57563700	H -4.26666300 -1.51000700 2.55407300
H 1.86529500 3.80995300 2.45376200	H 1.99175600 3.83368300 2.40232000
H -2.62782600 -0.87705800 2.86704000	H -2.61282400 -0.98591400 2.87859400
H 0.83598200 2.42053300 2.82616700	H 0.96384500 2.45813200 2.82391200
H -3.12739000 -2.45740900 3.48280700	H -3.16605700 -2.57699900 3.41554200
H 2.46228400 2.53652900 3.50756500	H 2.61349700 2.56509900 3.44724200
C -3.59422100 -3.67186800 1.02189700	C -3.66175500 -3.65780900 0.90340500
C 3.86108000 2.46875200 1.09400100	C 3.92160600 2.47840900 0.98201800
H -3.26682900 -4.17469000 0.10905200	H -3.34531600 -4.13310000 -0.02771600
H 4.31614900 1.91161200 0.27304900	H 4.35177700 1.90662900 0.15799400
H -4.64852800 -3.40950400 0.90620000	H -4.70515300 -3.35317300 0.79262200
H 3.87198300 3.53089100 0.83712700	H 3.91544100 3.53479400 0.70209400
H -3.53378000 -4.40063200 1.83571200	H -3.63247000 -4.42157700 1.68611300
H 4.50697000 2.34549700 1.96852200	H 4.59834600 2.37813500 1.83579900
H 0.37179400 -0.75528800 1.30966600	H 0.33604100 -0.72535000 1.32810100

H 0.79559600	-1.39675300	-0.65799600	H 0.77218000	-1.39482100	-0.67563000
C 0.97480000	-1.71294700	1.68732600	C 0.92383100	-1.71176600	1.71874100
H -5.18003300	-0.47959200	-2.63615600	H -5.07106900	-0.23388900	-2.66260900
H -3.61419600	0.30284800	-2.46140800	H -3.50902800	0.51961800	-2.36198400
H -3.71154800	-1.41760800	-2.87310200	H -3.59912700	-1.16025600	-2.92230200
H 1.10969800	4.61477000	-2.70333300	H 0.94809600	4.51595900	-2.76700400
H 1.80771900	3.00804000	-2.86371500	H 1.63033700	2.90297100	-2.93251500
H 0.07503400	3.20139800	-2.54286000	H -0.07238600	3.11108800	-2.47965500
H 0.22216400	-2.21076700	2.29909400	H 0.14408100	-2.17199100	2.32516900
C 1.54509000	-2.54145000	0.63896800	C 1.48433600	-2.56845900	0.69951800
H 0.96078400	-3.40144300	0.32136500	H 0.87721200	-3.40640900	0.36687600
N -1.58140300	1.49152900	1.61947900	Mo -0.84012100	0.64233000	0.16224600
Mo -0.84681600	0.62134600	0.20218400	C -1.46816400	1.40747900	1.87641300
C -1.78795500	1.76036800	-1.06337200	N -1.80724100	1.82495400	-0.78178400
H 1.70258700	-1.25472300	2.35930600	H 1.64882200	-1.24918500	2.39045700
C 2.93182100	-2.58556600	0.28336700	C 2.86259400	-2.61942000	0.31820700
C 3.38979900	-3.52123500	-0.68018600	C 3.29875700	-3.55668400	-0.65420200
C 3.92624700	-1.74049200	0.83324900	C 3.87173700	-1.78203400	0.85368900
C 4.71321700	-3.59261200	-1.06680900	C 4.61590600	-3.63785100	-1.06030900
H 2.66873000	-4.20542800	-1.11924100	H 2.56614200	-4.23502000	-1.08314200
C 5.25408900	-1.81781100	0.43898700	C 5.19273600	-1.86940200	0.43980400
H 3.65951900	-1.03199000	1.61011400	H 3.62181300	-1.07407100	1.63661800
C 5.66888800	-2.73507600	-0.51953800	C 5.58615900	-2.78864300	-0.52617300
H 5.01102400	-4.33038000	-1.80581200	H 4.89687300	-4.37650900	-1.80499100
H 5.98037400	-1.15457000	0.89954900	H 5.93105900	-1.21264600	0.89040300
H 6.70757500	-2.79296500	-0.82270700	H 6.61975900	-2.85418200	-0.84472000
2Mo-cis + PhCHCH₂-TS-H_N transfer			2Mo-trans + PhCHCH₂-TS-H_N transfer		
O -2.41453900	2.46877000	-1.72713500	O -2.51152200	2.59828300	-1.31989900
P 1.26766200	1.90783600	-0.06218400	P 1.28202400	1.89253700	-0.07869500
P -2.48577900	-1.26272900	-0.05817800	P -2.48316300	-1.26116200	-0.06659900
C 2.22591700	0.79753900	-1.20846300	C 2.23936300	0.78040600	-1.22743700
C -1.57254300	-2.38033400	-1.23756900	C -1.58090700	-2.38570200	-1.25166600
H 2.83342200	0.14084600	-0.57976300	H 2.85966100	0.13148000	-0.60294400
H -1.04089100	-3.10739700	-0.61958100	H -1.06255400	-3.12870900	-0.64106100
H 2.91401300	1.36009900	-1.84289400	H 2.91485700	1.34633300	-1.87299000
H -2.25284600	-2.93970800	-1.88331200	H -2.26844000	-2.92676200	-1.90583200
C 1.28977500	-0.05154700	-2.05408600	C 1.29974500	-0.07809800	-2.05878300
C -0.56471700	-1.59801900	-2.06737100	C -0.56058200	-1.60881500	-2.07058700
H 1.87995200	-0.81670500	-2.57628600	H 1.88770500	-0.85221100	-2.57058600
H 0.08840100	-2.30654600	-2.59678000	H 0.09227700	-2.32140900	-2.59521800
H 0.79346000	0.55493200	-2.81756800	H 0.80572200	0.51913700	-2.83108800
H -1.07217000	-0.99759000	-2.82781600	H -1.05785200	-1.00523700	-2.83548600
N 0.25868500	-0.70897000	-1.22266300	N 0.26163500	-0.72000500	-1.22426400
C -2.77637400	-2.42376500	1.39508900	C -2.83250400	-2.45124800	1.35068100
C 2.42566400	2.02746200	1.41423400	C 2.48302100	2.06005900	1.35922700
H -1.75086900	-2.74508300	1.60765000	H -1.81732000	-2.78275500	1.59615600
H 2.50470900	0.97199300	1.69460200	H 2.57746100	1.01352400	1.66820600
C -4.17956900	-1.00305700	-0.83077600	C -4.14140800	-0.93421200	-0.88424100
C 1.29842800	3.60965100	-0.85973700	C 1.25630600	3.56659900	-0.92882900
C -4.09374400	-0.67829200	-2.32062700	C -3.98205800	-0.51926200	-2.34581600
C 1.01055200	3.55259700	-2.35854100	C 0.85067600	3.45193200	-2.39719500
O -2.02851500	2.00132300	2.58089000	O -1.82541000	1.79946700	2.91344900
H 2.32053700	3.97805800	-0.72235800	H 2.28908700	3.92935700	-0.88654000
H -4.70332600	-1.95827700	-0.72070200	H -4.67487000	-1.89041500	-0.85668300
C 0.32915300	4.56300300	-0.16208000	C 0.35106500	4.55617600	-0.19648000
C -4.95834000	0.07950700	-0.08527900	C -4.94736800	0.10771400	-0.11022600
H 0.52691600	4.65917500	0.90546600	H 0.63540900	4.69548700	0.84622600
H -5.09102000	-0.15069400	0.97213900	H -5.12526700	-0.18325600	0.92509100
H -0.70216100	4.22663800	-0.27931100	H -0.68881000	4.22833500	-0.21960200
H -4.45105100	1.04334900	-0.15412400	H -4.43886900	1.07263700	-0.10457600
H 0.40869300	5.55984500	-0.60591900	H 0.40431000	5.53257300	-0.68742600
H -5.95265100	0.19104400	-0.52763800	H -5.92217600	0.24568700	-0.58737100

C -3.29837000	-1.71008700	2.63969500	C -3.40618900	-1.77470200	2.59271300
C 1.81716600	2.77359500	2.59917000	C 1.92094300	2.84110700	2.54412800
H -4.35064800	-1.43645600	2.53798300	H -4.45759700	-1.51162900	2.45991100
H 1.80466700	3.85282200	2.43240400	H 1.91736100	3.91608300	2.35229600
H -2.73311600	-0.80325700	2.85848100	H -2.86130800	-0.86772700	2.85516700
H 0.79701900	2.44980000	2.80977000	H 0.90458400	2.53658400	2.79513000
H -3.22165100	-2.37380500	3.50586800	H -3.35199400	-2.45994800	3.44363400
H 2.41916500	2.59536300	3.49496400	H 2.54936600	2.67546300	3.42399800
C -3.60338100	-3.66432100	1.06761200	C -3.64909500	-3.67928000	0.95513000
C 3.82560400	2.53869000	1.08519500	C 3.86829300	2.56501800	0.96319200
H -3.23839800	-4.19218900	0.18372900	H -3.24495200	-4.19002500	0.07870500
H 4.29134800	1.98687800	0.26657600	H 4.31106100	1.98335500	0.15289700
H -4.65519900	-3.41667200	0.90572500	H -4.69017600	-3.42000500	0.74822600
H 3.81757500	3.59984900	0.82422200	H 3.84312600	3.61465600	0.65977800
H -3.56565300	-4.36592100	1.90632400	H -3.65626900	-4.39927000	1.77883700
H 4.47234600	2.43040800	1.96108900	H 4.54410100	2.49624300	1.82084500
H 0.39914800	-0.76310400	1.40167000	H 0.38808400	-0.76493600	1.41314100
H 0.86914700	-1.45633800	-0.55202700	H 0.86642300	-1.47303100	-0.54051200
C 1.00975600	-1.70952200	1.67574300	C 0.98623900	-1.72496900	1.68319900
H -5.10373000	-0.54772800	-2.72024900	H -4.97033100	-0.34164200	-2.77996400
H -3.55145700	0.25075000	-2.50060800	H -3.41321300	0.40667500	-2.44149300
H -3.61887300	-1.47411800	-2.89728400	H -3.49781200	-1.28945300	-2.94881700
H 1.04547400	4.56467800	-2.77243000	H 0.85090600	4.44747000	-2.85070500
H 1.74192600	2.95413500	-2.90430700	H 1.53948900	2.83274400	-2.97430300
H 0.01524900	3.15418800	-2.56140100	H -0.15664600	3.04596300	-2.50431300
H 0.30421000	-2.28876900	2.27346400	H 0.26320800	-2.29813400	2.26559200
C 1.54909600	-2.43150800	0.50669100	C 1.52972600	-2.44189200	0.51514400
H 1.01576700	-3.34810200	0.25724600	H 0.99941100	-3.35947800	0.26278900
N -1.57585600	1.46772000	1.63341500	Mo -0.85722100	0.62337900	0.16575800
Mo -0.85163200	0.60947200	0.19930800	C -1.46902100	1.36719600	1.90107600
C -1.82190300	1.75943400	-1.02301300	N -1.85410000	1.80817200	-0.72951500
H 1.76583400	-1.31499300	2.35750100	H 1.73572200	-1.34229800	2.37896200
C 2.97012700	-2.52549300	0.23449800	C 2.95341200	-2.53312800	0.25002300
C 3.44291800	-3.45991900	-0.71636000	C 3.43238500	-3.46152900	-0.70312000
C 3.95457300	-1.71571000	0.83924600	C 3.93274700	-1.72451000	0.86359900
C 4.78095800	-3.56334900	-1.04552700	C 4.77245600	-3.56112500	-1.02576600
H 2.72425600	-4.11863600	-1.19635500	H 2.71737600	-4.11896000	-1.19028100
C 5.29873800	-1.82159500	0.50534400	C 5.27905500	-1.82629200	0.53640300
H 3.67057100	-1.00402200	1.60709500	H 3.64306100	-1.01740300	1.63360800
C 5.73110200	-2.73866200	-0.44346000	C 5.71787500	-2.73786200	-0.41459300
H 5.09290000	-4.30048300	-1.77910600	H 5.08950100	-4.29387900	-1.76153700
H 6.01960600	-1.18156800	1.00519000	H 5.99614200	-1.18741200	1.04309100
H 6.78083300	-2.82090200	-0.69992900	H 6.76907200	-2.81699700	-0.66602100
2Mo-cis + CN-Ph-CHCH2-TS-H_M transfer (CN bond)			2Mo-cis + CN-Ph-CHCH2-TS-H_M transfer (C=C bond)		
C -3.01475100	0.00035300	0.79157800	O -3.00550600	1.90923600	-2.09351500
O -4.13864300	0.00046300	1.08366100	P 0.51375300	2.22430300	0.01792200
Mo -1.08096600	0.00008500	0.32932500	P -2.38948900	-1.68503000	-0.13624800
P -1.02512100	2.43509500	-0.16977200	C 1.74441400	1.38519500	-1.11423100
P -1.02578100	-2.43492000	-0.16981200	C -1.22865200	-2.54564600	-1.32850700
C -1.35990700	2.44815500	-2.00870000	H 2.45049600	0.84808300	-0.47497100
C -1.36038500	-2.44782400	-2.00877000	H -0.53771900	-3.13678100	-0.72092500
H -0.38278100	2.41278500	-2.49867000	H 2.32442400	2.10659400	-1.69351000
H -0.38320200	-2.41260600	-2.49863800	H -1.75712900	-3.24318000	-1.98152200
H -1.85423900	3.36668200	-2.33064900	C 1.05612000	0.39832300	-2.04542400
H -1.85485500	-3.36624100	-2.33082100	C -0.43940000	-1.54204800	-2.15629000
C -2.16455100	1.22682400	-2.42836700	H 1.81027600	-0.16274200	-2.61327500
C -2.16475900	-1.22631800	-2.42844500	H 0.32364700	-2.06549800	-2.74882300
H -2.24729200	1.19906500	-3.52382000	H 0.42160200	0.92042300	-2.76507100
H -2.24743300	-1.19850600	-3.52390200	H -1.09397000	-1.01535200	-2.85396300
H -3.17784100	1.26314000	-2.02163900	N 0.19371400	-0.53104800	-1.28802700
H -3.17808000	-1.26244800	-2.02177800	C -2.38891400	-2.90621600	1.29828500
N -1.51003200	0.00018200	-1.93985700	C 1.57082700	2.53012200	1.54400800

C 0.61700300	-3.34564500	-0.09134900	H -1.31265000	-3.03154700	1.45757400
C 0.61791300	3.34538400	-0.09146900	H 1.93598200	1.51580000	1.73443400
H 1.26360700	-2.65598300	-0.64415400	C -4.09156200	-1.86678800	-0.91753700
H 1.26425800	2.65559500	-0.64442000	C 0.24943900	3.92753300	-0.73670900
C -2.26749000	-3.63007700	0.58890300	C -4.09810200	-1.51596700	-2.40337900
C -2.26643600	3.63056600	0.58909600	C 0.03632100	3.87490200	-2.24783400
C -3.65705800	-3.50920300	-0.03212900	O -2.99836100	1.69836100	2.30395400
C -3.65610500	3.51005100	-0.03178000	H 1.16955200	4.48810100	-0.54290700
N -0.56808900	-0.00000200	2.06663500	H -4.35796600	-2.92368900	-0.81693200
O -0.20636200	-0.00006300	3.19136500	C -0.91957200	4.63593400	-0.05386500
C -2.34224700	3.42259800	2.10159400	C -5.11295100	-1.01999800	-0.16004900
C -2.34342100	-3.42209600	2.10139500	H -0.76974500	4.75537600	1.01966300
H -1.37408400	3.52781400	2.59159800	H -5.19066200	-1.29750500	0.89190300
H -1.37532700	-3.52747900	2.59149900	H -1.84840500	4.08064000	-0.19861100
H -2.72147600	2.42596200	2.33469600	H -4.84883100	0.03860900	-0.20481500
H -2.72249800	-2.42539300	2.33445600	H -1.05189300	5.63345600	-0.48310800
H -3.02269300	4.15658700	2.54392600	H -6.10337800	-1.14078700	-0.60856500
H -3.02404200	-4.15596500	2.54365600	C -2.97208900	-2.30664200	2.57527600
C 1.15491100	-3.44742600	1.33392100	C 0.74629200	2.95079500	2.75771300
C 1.15605600	3.44691000	1.33373000	H -4.05841000	-2.21035500	2.51958900
H 0.61852900	-4.20523000	1.91025500	H 0.39459700	3.98106500	2.67240500
H 0.61997200	4.20482600	1.91019500	H -2.55724700	-1.31835300	2.77975400
H 1.08167500	-2.49818100	1.86707500	H -0.12227400	2.30567600	2.89669800
H 1.08262500	2.49764700	1.86682500	H -2.74989600	-2.95560700	3.42769800
H 2.20787700	-3.74231500	1.31354400	H 1.36083400	2.89558000	3.66130400
H 2.20910300	3.74150000	1.31322600	C -2.98390800	-4.27757400	0.99093800
C 0.64007000	-4.70193200	-0.79132900	C 2.77445900	3.44328500	1.32993600
C 0.64124600	4.70171900	-0.79134700	H -2.58196800	-4.71549600	0.07398500
H 0.30273700	-4.64638700	-1.82816000	H 3.37851200	3.14936700	0.46849800
H 0.30359800	4.64637700	-1.82808700	H -4.07143700	-4.23346600	0.89676800
H 0.02147700	-5.43835200	-0.27182000	H 2.47220400	4.48430300	1.19336600
H 0.02305400	5.43830400	-0.27159800	H -2.76207100	-4.96989500	1.80868300
H 1.66182100	-5.09360000	-0.80177500	H 3.42363900	3.41402200	2.21036300
H 1.66312900	5.09303800	-0.80205300	H -0.05934500	-0.37346100	1.30193700
H 0.63680400	-0.00035700	-0.43708300	H 0.78312300	-1.02943800	-0.61172000
H -0.54889500	0.00011700	-2.33538800	C 0.99449800	-1.43046800	2.03503900
N 1.25043700	0.00001900	-2.77183300	H -5.10736300	-1.65501500	-2.80214100
C 1.72847500	-0.00014100	-1.69119300	H -3.82275600	-0.47478000	-2.57362600
C 2.97360500	-0.00028500	-0.93140900	H -3.43188900	-2.15209800	-2.98982800
C 3.02759100	-0.00043000	0.45670400	H -0.10332100	4.89114600	-2.62815200
C 4.25237900	-0.00056900	1.10536200	H 0.88964800	3.44853200	-2.77890300
C 5.45583500	-0.00057400	0.39408000	H -0.85680400	3.30617700	-2.50982700
C 4.17260800	-0.00027200	-1.66056500	H 0.14667000	-1.85303000	2.55564400
C 5.38749300	-0.00040600	-1.00692200	C 1.74021800	-2.23296900	1.20146200
H 2.09573900	-0.00043000	1.01018000	H 1.29974000	-3.17041200	0.87085800
H 4.27821200	-0.00068900	2.19021700	N -2.33301100	1.24553800	1.44336000
H 4.12762100	-0.00015400	-2.74317800	Mo -1.28913100	0.52517400	0.14968200
H 6.29828500	-0.00034700	-1.59430700	C -2.35659000	1.37740200	-1.29083500
H -1.88398700	4.63650000	0.38581200	H 1.45463000	-0.60185300	2.56013600
H -1.88527800	-4.63610900	0.38566200	C 3.07260900	-1.97925300	0.71656000
H -4.33587200	-4.21546300	0.45520900	C 3.65810600	-2.86285900	-0.21676600
H -4.33467200	4.21651500	0.45560800	C 3.86957000	-0.89440800	1.14270800
H -4.07241300	-2.51017000	0.11202400	C 4.93254100	-2.67304400	-0.70549100
H -4.07171500	2.51113600	0.11245200	H 3.08505500	-3.72064800	-0.55426200
H -3.66458200	-3.73817400	-1.09945700	C 5.14543700	-0.69667600	0.65873300
H -3.66368600	3.73898400	-1.09911400	H 3.48769100	-0.20893200	1.88980400
C 6.71915000	-0.00070800	1.13581000	C 5.69765300	-1.57793500	-0.28103700
H 6.60702300	-0.00106100	2.21783700	H 5.35135000	-3.36996500	-1.42207400
C 7.95362500	-0.00047900	0.63295500	H 5.73586200	0.14118300	1.01119800
H 8.15489300	-0.00017900	-0.43255100	C 7.00874900	-1.36752500	-0.78819800
H 8.81773100	-0.00060400	1.28622900	N 8.07286500	-1.19252900	-1.20490900
2Mo-<i>cis</i> + CN-Ph-CHCH2-interm (CN bond)			2Mo-<i>cis</i> + CN-Ph-CHCH2-interm (C=C bond)		

C	-2.97531000	0.00078700	-0.79222200	O	-3.00756600	2.02608100	-1.89067900
O	-4.09528300	0.00108900	-1.09845500	P	0.61612900	2.16873100	-0.01959500
Mo	-1.07522600	0.00024500	-0.31379000	P	-2.50706800	-1.62709700	-0.11638700
P	-1.02525700	-2.44787300	0.17680700	C	1.79615700	1.24103500	-1.12582000
P	-1.02378200	2.44831300	0.17689600	C	-1.38744900	-2.54941700	-1.29243000
C	-1.27200900	-2.45141200	2.02583400	H	2.48095100	0.69106100	-0.47361800
C	-1.27050400	2.45190500	2.02592800	H	-0.74262200	-3.17995100	-0.67538100
H	-0.27138300	-2.41971600	2.46565000	H	2.40504200	1.91670700	-1.72981900
H	-0.26989400	2.41958300	2.46572500	H	-1.94778600	-3.21229200	-1.95475200
H	-1.75786800	-3.36457600	2.37503100	C	1.05515800	0.25882600	-2.01840200
H	-1.75581100	3.36534900	2.37516900	C	-0.52590300	-1.59340900	-2.10332100
C	-2.04088300	-1.21872800	2.47716600	H	1.78126200	-0.36460800	-2.55486200
C	-2.04013600	1.21967800	2.47720200	H	0.22793200	-2.16385500	-2.66185700
H	-2.04590500	-1.17734900	3.57525800	H	0.45445900	0.78416600	-2.76444300
H	-2.04519400	1.17826900	3.57529300	H	-1.12949500	-1.04770900	-2.83200000
H	-3.08211300	-1.25781100	2.14663700	N	0.14446600	-0.60410400	-1.22999900
H	-3.08133900	1.25942400	2.14666500	C	-2.59375400	-2.83761800	1.32280900
N	-1.41118700	0.00029200	1.93656700	C	1.68223600	2.49144400	1.49398900
C	0.60995100	3.36427400	0.01828500	H	-1.52897600	-2.98359400	1.53463700
C	0.60793500	-3.36480000	0.01820500	H	1.95260500	1.46835300	1.77416100
H	1.28646600	2.68415600	0.54718000	C	-4.21064400	-1.67415500	-0.90814000
H	1.28483100	-2.68510900	0.54715500	C	0.37514300	3.84842000	-0.82725100
C	-2.31248800	3.62279300	-0.52834100	C	-4.17329800	-1.34740700	-2.39931300
C	-2.31465300	-3.62156900	-0.52845100	C	0.16865000	3.74986800	-2.33715200
C	-3.67424400	3.47230600	0.14587500	O	-2.81944500	1.73393400	2.42155500
C	-3.67630800	-3.47031400	0.14580400	H	1.30756300	4.39306000	-0.64658800
N	-0.57829700	0.00011300	-2.06056100	H	-4.55761500	-2.70611400	-0.79434100
O	-0.23516000	-0.00001200	-3.18833700	C	-0.77836500	4.60864200	-0.17406500
C	-2.44398000	-3.43021400	-2.03943600	C	-5.17253900	-0.74217000	-0.17284300
C	-2.44189300	3.43158800	-2.03933400	H	-0.64407700	4.73869300	0.89981100
H	-1.49620800	-3.55340500	-2.56365000	H	-5.26833600	-0.98633500	0.88554300
H	-1.49403000	3.55421600	-2.56351300	H	-1.72612200	4.09084000	-0.33007300
H	-2.82244500	-2.43347900	-2.27257000	H	-4.84329800	0.29594800	-0.24569400
H	-2.82099200	2.43511500	-2.27255700	H	-0.86315300	5.60366200	-0.62044100
H	-3.14832600	-4.16205300	-2.44619900	H	-6.16830000	-0.81083600	-0.62010000
H	-3.14576500	4.16390300	-2.44606400	C	-3.23111900	-2.23357100	2.57159700
C	1.08750500	3.46671600	-1.42834800	C	0.90265000	3.09649200	2.65898800
C	1.08551100	-3.46748900	-1.42840400	H	-4.31309100	-2.13187800	2.46535700
H	0.52483100	4.22164600	-1.98279400	H	0.68338900	4.15318900	2.49276000
H	0.52238400	-4.22203800	-1.98290700	H	-2.82124800	-1.24965200	2.80437100
H	0.99919900	2.51737100	-1.95890400	H	-0.04013700	2.57722000	2.83736100
H	0.99785300	-2.51807000	-1.95892600	H	-3.05256200	-2.88641700	3.43074500
H	2.13888300	3.76628800	-1.45008500	H	1.50017800	3.03386400	3.57287200
H	2.13669900	-3.76773400	-1.45008300	C	-3.19813200	-4.19712300	0.98098200
C	0.65125600	4.72246200	0.71408200	C	2.96849300	3.26350300	1.21283000
C	0.64839200	-4.72303500	0.71396900	H	-2.75412800	-4.64377100	0.08852700
H	0.35590200	4.66652700	1.76342500	H	3.55612000	2.82183400	0.40581500
H	0.35302900	-4.66693700	1.76330100	H	-4.27786700	-4.13212300	0.82780600
H	0.00817300	5.45358300	0.21738900	H	2.76725600	4.30721800	0.95984300
H	0.00487800	-5.45375700	0.21724600	H	-3.03430900	-4.89217000	1.80965400
H	1.67031800	5.11945100	0.68322200	H	3.59717800	3.26814000	2.10803400
H	1.66720800	-5.12065500	0.68314300	H	0.15125700	-0.56255200	1.40777200
H	0.75573400	-0.00025500	0.52232100	H	0.75895700	-1.16659200	-0.57476000
H	-0.39769700	-0.00002500	2.32166500	C	0.86612800	-1.37946700	1.85811800
N	1.21890500	-0.00051200	2.62848400	H	-5.18723800	-1.40470200	-2.80557500
C	1.59110800	-0.00056800	1.47063000	H	-3.80829600	-0.33629500	-2.58278700
C	2.92103800	-0.00093400	0.82064700	H	-3.55929000	-2.04754800	-2.96881800
C	3.05640600	-0.00084800	-0.56198600	H	0.05141500	4.75560800	-2.75084500
C	4.31453600	-0.00123200	-1.14566200	H	1.01504800	3.28832500	-2.84867900
C	5.47478400	-0.00160100	-0.36594200	H	-0.73565300	3.19206400	-2.58516200
C	4.07494600	-0.00147000	1.61344200	H	0.18253900	-1.97323500	2.46556300
C	5.32541000	-0.00183400	1.02974700	C	1.61979300	-2.15709500	0.87775100
H	2.16267100	-0.00051500	-1.17874700	H	1.18303900	-3.09852600	0.55503000

H 4.40348100 -0.00115700 -2.22751300	N -2.21352500 1.26788100 1.52894600
H 3.95865100 -0.00167000 2.69129600	Mo -1.25449100 0.51900400 0.17949300
H 6.20314500 -0.00246800 1.66605100	C -2.33862800 1.44593400 -1.13990900
H -1.94134700 -4.63147300 -0.32793900	H 1.48169200 -0.78671400 2.53707800
H -1.93858500 4.63247400 -0.32778700	C 2.98506400 -1.97504000 0.55861100
H -4.38220600 4.17356400 -0.30568500	C 3.63870400 -2.86379200 -0.34631600
H -4.38470600 -4.17109800 -0.30580500	C 3.80232900 -0.93209800 1.08105500
H -4.08032900 2.46877900 0.00667100	C 4.95069700 -2.70995100 -0.71369100
H -4.08178500 -2.46653200 0.00669300	H 3.07021100 -3.69427500 -0.75441300
H -3.64191600 3.68864500 1.21520400	C 5.12130100 -0.77936200 0.71497600
H -3.64408800 -3.68677100 1.21511200	H 3.39461600 -0.24950800 1.81791600
C 6.77846600 -0.00175300 -1.03386000	C 5.72750300 -1.65204900 -0.20082300
H 6.72784600 -0.00388700 -2.12079200	H 5.40392700 -3.41009700 -1.40680400
C 7.98386100 0.00063800 -0.46406900	H 5.70934800 0.02345700 1.14650300
H 8.12565500 0.00311900 0.61095100	C 7.07834300 -1.47953600 -0.58929100
H 8.88256700 0.00026000 -1.06895600	N 8.18124600 -1.33381600 -0.91165800
2Mo-cis + CN-Ph-CHCH2-TS-H_N transfer (CN bond)	2Mo-cis + CN-Ph-CHCH2-TS-H_N transfer (C=C bond)
C -3.01615200 0.00021900 0.74313900	O -3.13937200 2.00204400 -1.78521700
O -4.14223100 0.00030700 1.02592400	P 0.55488400 2.19435800 -0.05223600
Mo -1.11871300 0.00006100 0.30160300	P -2.49604100 -1.66724300 -0.09984400
P -1.05213000 2.45191500 -0.17598200	C 1.76429300 1.27132800 -1.12481100
P -1.05253100 -2.45178500 -0.17602200	C -1.33001100 -2.60393500 -1.21180900
C -1.13760300 2.45731900 -2.03696000	H 2.46840700 0.77462600 -0.45239300
C -1.13771100 -2.45710000 -2.03700800	H -0.70484600 -3.21371000 -0.55610400
H -0.10251200 2.44987300 -2.38834500	H 2.34643600 1.94609500 -1.75601400
H -0.10256200 -2.44968500 -2.38822400	H -1.86213000 -3.28766000 -1.87673100
H -1.61103800 3.36201100 -2.42400500	C 1.05573600 0.22418200 -1.97024200
H -1.61112100 -3.36175500 -2.42417100	C -0.44920800 -1.65409800 -2.01142100
C -1.83944200 1.20801700 -2.55072500	H 1.81082700 -0.42503500 -2.43455600
C -1.83940200 -1.20774200 -2.55083800	H 0.36029600 -2.23115300 -2.48168900
H -1.70998800 1.15310300 -3.64173900	H 0.49520800 0.69670600 -2.78342400
H -1.70977100 -1.15280400 -3.64182900	H -1.02031800 -1.19067400 -2.82224900
H -2.91690600 1.25828700 -2.36001300	N 0.13112500 -0.59602900 -1.16140600
H -2.91689900 -1.25795800 -2.36029900	C -2.60749900 -2.82921200 1.37763400
N -1.27629200 0.00011700 -1.92556900	C 1.60218700 2.57779700 1.46206900
C 0.56041900 -3.37019300 0.12708900	H -1.54616500 -2.95433900 1.61971800
C 0.56103600 3.37002400 0.12688600	H 1.91813800 1.56907800 1.74904800
H 1.27301800 -2.71323500 -0.38398000	C -4.16775300 -1.77005000 -0.95003500
H 1.27340600 2.71305400 -0.38448600	C 0.28488400 3.84172800 -0.91335200
C -2.40795300 -3.61581000 0.40752000	C -4.08095300 -1.42342000 -2.43487700
C -2.40723800 3.61617000 0.40783000	C 0.02707500 3.67353600 -2.40926800
C -3.71676600 -3.40620800 -0.35084600	O -2.77310900 1.64634100 2.50012200
C -3.71620000 3.40689900 -0.35036700	H 1.22443700 4.39045900 -0.78989300
N -0.66955300 -0.00000100 2.06587400	H -4.47505100 -2.81735600 -0.86261300
O -0.34767200 -0.00004800 3.20008600	C -0.84361300 4.63400200 -0.25549800
C -2.63261000 3.47532800 1.91275300	C -5.19808000 -0.88912900 -0.24577000
C -2.63350900 -3.47504400 1.91242200	H -0.66108300 4.82876400 0.80134200
H -1.72833800 3.65626100 2.49384100	H -5.34058400 -1.16339800 0.79981400
H -1.72938100 -3.65631000 2.49362700	H -1.79455800 4.10496800 -0.33747800
H -2.98974400 2.47408400 2.15986200	H -4.90385900 0.16147200 -0.27765800
H -2.99037900 -2.47371700 2.15957500	H -0.95497400 5.60054900 -0.75543700
H -3.38961200 4.19329500 2.24221600	H -6.16629100 -0.98088000 -0.74632700
H -3.39078000 -4.19281300 2.24170000	C -3.28083900 -2.19824400 2.59383900
C 0.95091300 -3.41941900 1.60233400	C 0.80064900 3.15400600 2.62677600
C 0.95191300 3.41892600 1.60203800	H -4.36084000 -2.11081800 2.46003900
H 0.35623700 -4.15392400 2.15025500	H 0.53111100 4.19794700 2.45505900
H 0.35740300 4.15332700 2.15027600	H -2.88714200 -1.20466500 2.81073700
H 0.83154700 -2.45190000 2.09217500	H -0.11624800 2.59386200 2.81354800
H 0.83263900 2.45130300 2.09169400	H -3.11611300 -2.82666300 3.47385900
H 1.99874800 -3.71764900 1.69712900	H 1.40485100 3.12564500 3.53813100
H 1.99978300 3.71709800 1.69662800	C -3.18745400 -4.20564900 1.06229000
C 0.63737100 -4.75248800 -0.51637500	C 2.85247700 3.40472300 1.17418600

C 0.63802700	4.75242500	-0.51634900	H -2.71349200	-4.67448500	0.19701500
H 0.39600400	-4.73452700	-1.58097000	H 3.45347200	2.99015100	0.36243700
H 0.39608900	4.73474600	-1.58082000	H -4.26285400	-4.15630200	0.87603000
H -0.03152800	-5.46499000	-0.02698400	H 2.60279400	4.43815300	0.92219200
H -0.03041900	5.46500700	-0.02645800	H -3.04126000	-4.87286000	1.91684200
H 1.65294300	-5.14762900	-0.41859600	H 3.48597300	3.43798600	2.06550100
H 1.65375800	5.14727000	-0.41903000	H 0.18319800	-0.56135200	1.52920200
H 0.85479500	-0.00015800	-0.40421100	H 0.87729700	-1.21704500	-0.40852200
H -0.10769700	0.00014900	-2.28052300	C 0.95152600	-1.35321100	1.82102300
N 1.25099500	0.00012100	-2.48079200	H -5.07315700	-1.51775700	-2.88557300
C 1.63876500	-0.00006300	-1.31218400	H -3.75012700	-0.39616400	-2.59126800
C 2.99909700	-0.00021300	-0.73520000	H -3.41282900	-2.08971000	-2.98341000
C 3.19468100	-0.00040800	0.64170300	H -0.10803600	4.65863700	-2.86511500
C 4.47707900	-0.00056700	1.16995700	H 0.85710900	3.18924100	-2.92631900
C 5.60172900	-0.00050600	0.33958700	H -0.88185200	3.10113300	-2.59946400
C 4.11737900	-0.00019500	-1.57703300	H 0.38054400	-2.05813600	2.42770800
C 5.39183200	-0.00034700	-1.04846900	C 1.63144000	-1.98140300	0.65394100
H 2.33140000	-0.00044200	1.30065000	H 1.27665800	-2.98686000	0.42760900
H 4.61388900	-0.00071600	2.24673800	N -2.19870300	1.20928500	1.57137700
H 3.95368400	-0.00008200	-2.64873800	Mo -1.27189900	0.49772700	0.17350800
H 6.24131800	-0.00038700	-1.72195600	C -2.43100500	1.42956800	-1.06563200
H -2.04397900	4.62703000	0.19408600	H 1.62096700	-0.81793200	2.49684600
H -2.04487400	-4.62672800	0.19374000	C 3.05259600	-1.85361500	0.43724500
H -4.46916300	-4.10647600	0.02389300	C 3.71100100	-2.73478900	-0.45712100
H -4.46839300	4.10730800	0.02451700	C 3.86621000	-0.86126600	1.03144500
H -4.10866700	-2.39876200	-0.20125100	C 5.04875800	-2.62313000	-0.75239800
H -4.10830000	2.39953000	-0.20078000	H 3.13358100	-3.52836000	-0.92171000
H -3.61472900	-3.58242300	-1.42301000	C 5.21114400	-0.74321200	0.74118400
H -3.61427500	3.58315600	-1.42253500	H 3.44031900	-0.17726800	1.75649100
C 6.93363900	-0.00062600	0.94921400	C 5.82967900	-1.61408400	-0.16285900
H 6.93163500	-0.00139000	2.03728200	H 5.51331600	-3.31929200	-1.44154100
C 8.11219000	0.00015800	0.32586000	H 5.80216000	0.02733700	1.22356600
H 8.20569800	0.00102600	-0.75443200	C 7.20996300	-1.48670400	-0.46869500
H 9.03718700	-0.00002100	0.88969600	N 8.33392900	-1.37976500	-0.72135900
Fe + CN-Ph-CHCH2-TS-H_M transfer (CN bond)			Fe + CN-Ph-CHCH2-TS-H_M transfer (C=C bond)		
P -1.24727700	2.20307900	-0.05323200	P -0.14333600	2.10238400	0.11319700
P -1.24933800	-2.20244500	-0.05334900	P 2.47040400	-1.42770400	0.19211300
C -1.62706600	2.44585000	-1.85917300	C -1.48896000	1.46404600	1.23501100
C -1.62910000	-2.44476900	-1.85935500	C 1.45780500	-2.48174600	1.35223700
H -0.66465700	2.53426600	-2.37093900	H -2.28132600	1.06375300	0.59729000
H -0.66669800	-2.53396300	-2.37100100	H 0.85912900	-3.15596800	0.73348600
H -2.19776000	3.35420400	-2.06242700	H -1.93221100	2.24544200	1.85624400
H -2.20053600	-3.35262600	-2.06275100	H 2.07050700	-3.10113800	2.01107000
C -2.35161000	1.20998000	-2.35388900	C -0.90400900	0.36038200	2.09361700
C -2.35254600	-1.20825200	-2.35406500	C 0.55376500	-1.56691600	2.15474500
H -2.42327600	1.21947000	-3.45010700	H -1.69942200	-0.18818500	2.61466900
H -2.42409200	-1.21759600	-3.45029100	H -0.20642400	-2.14648400	2.69588900
H -3.36692400	1.17024600	-1.95413500	H -0.23890200	0.78152300	2.84971900
H -3.36787600	-1.16771300	-1.95443200	H 1.13638400	-1.01347000	2.89319500
N -1.64358600	0.00055700	-1.90135800	N -0.08876900	-0.56580500	1.28101800
C 0.27369400	-3.29009500	0.14087200	C 2.73536000	-2.64427500	-1.22411900
C 0.27672100	3.28939600	0.14087500	C -1.16704600	2.68060600	-1.35917900
H 0.99760400	-2.74621900	-0.47614800	H 1.70576900	-2.97537300	-1.40249000
H 1.00015500	2.74484300	-0.47610700	H -1.76702900	1.78311900	-1.54543900
C -2.60897500	-3.11451400	0.87432600	C 4.14472900	-1.29611000	1.03771400
C -2.60599600	3.11629800	0.87468000	C 0.44940100	3.67994200	0.94663600
C -3.98807100	-2.87562600	0.26484800	C 4.01745100	-0.85352900	2.49278200
C -3.98536200	2.87885100	0.26525000	C 0.76843500	3.46272000	2.42328400
O -0.31051400	-0.00012800	2.85662700	O 2.94741100	1.60421600	-1.96982100
C -2.62162800	2.71849000	2.34976200	H -0.38184000	4.38885100	0.87530900
C -2.62430200	-2.71690100	2.34946500	H 4.56930700	-2.30513000	1.02123500
H -1.66315500	2.87372900	2.84516400	C 1.66495400	4.25811700	0.22565800

H -1.66599100	-2.87308200	2.84488400	C 5.07296000	-0.35017000	0.27911000
H -2.88011700	1.66275400	2.45081000	H 1.47262500	4.47035800	-0.82674800
H -2.88182900	-1.66094300	2.45065000	H 5.22706400	-0.64864500	-0.75860900
H -3.37362200	3.30678200	2.88472800	H 2.50624000	3.56447100	0.27831800
H -3.37685500	-3.30457800	2.88432200	H 4.67033700	0.66441400	0.27868400
C 0.81351700	-3.32728200	1.56850500	H 1.96879400	5.19516900	0.70190200
C 0.81657400	3.32621100	1.56850800	H 6.05325900	-0.32376900	0.76438300
H 0.18208000	-3.93830700	2.21826400	C 3.22580200	-1.98650100	-2.51095300
H 0.18562300	3.93776700	2.21823900	C -0.34515000	2.94102700	-2.61806700
H 0.89279000	-2.33334600	2.00869500	H 4.26132100	-1.64977600	-2.43053700
H 0.89506200	2.33223100	2.00874200	H 0.27945700	3.83166500	-2.52438200
H 1.81120300	-3.77588500	1.57461500	H 2.61481800	-1.12490800	-2.78053800
H 1.81461600	3.77402000	1.57459600	H 0.30464300	2.09871400	-2.85482500
C 0.12598800	-4.70413600	-0.41782400	H 3.18337100	-2.70560700	-3.33475900
C 0.13025000	4.70352800	-0.41791400	H -1.01383200	3.10472600	-3.46883500
H -0.19329900	-4.71478000	-1.46139400	C 3.56779000	-3.87424200	-0.86959900
H -0.18904400	4.71438300	-1.46147900	C -2.12139500	3.83475600	-1.06205700
H -0.58771300	-5.29647800	0.16109100	H 3.23081200	-4.35995000	0.04936600
H -0.58292100	5.29653600	0.16097100	H -2.72198900	3.66412600	-0.16563400
H 1.08805100	-5.22325700	-0.36617000	H 4.62487100	-3.62403000	-0.75168700
H 1.09277000	5.22180500	-0.36631100	H -1.58457300	4.77812500	-0.93583200
H 0.43219600	-0.00087300	-0.47923800	H 3.50123000	-4.61334200	-1.67376600
H -0.71371200	0.00024700	-2.36839000	H -2.81355700	3.97053200	-1.89864900
N 1.04777300	-0.00015500	-2.81488000	H 0.26086400	-0.33101800	-1.20170600
C 1.51408000	-0.00048500	-1.72809700	H -0.71241900	-1.06424800	0.63455900
C 2.76905200	-0.00084900	-0.98297500	C -0.79859600	-1.37354700	-1.96736200
C 2.84118200	-0.00114000	0.40399100	H 5.01377200	-0.75163200	2.93321400
C 4.07369400	-0.00148400	1.03836600	H 3.51664700	0.11497500	2.55814400
C 5.26838500	-0.00154700	0.31280300	H 3.46576200	-1.57137500	3.10368300
C 3.95967100	-0.00088800	-1.72581000	H 1.14835300	4.39268200	2.85672800
C 5.18251400	-0.00122100	-1.08721400	H -0.10895500	3.17004700	3.00390800
H 1.91731800	-0.00108800	0.96856900	H 1.53661900	2.69514600	2.54221700
H 4.11307200	-0.00172100	2.12289800	H 0.06117700	-1.83568600	-2.43181000
H 3.90113100	-0.00065300	-2.80772700	C -1.61341900	-2.13425200	-1.16282500
H 6.08607200	-0.00119100	-1.68577100	H -1.23058200	-3.08726400	-0.80580600
H -4.74625300	-3.39769600	0.85636500	H -1.19745900	-0.53225200	-2.52153800
H -4.74298600	3.40164100	0.85684700	C -2.95506500	-1.81558700	-0.74287700
H -4.23233300	-1.81050200	0.27603900	C -3.63335500	-2.67607200	0.14748200
H -4.23070200	1.81397400	0.27637100	C -3.66770300	-0.68332000	-1.19256400
H -4.06756700	-3.24087300	-0.76089900	C -4.91921300	-2.42245800	0.57354900
H -4.06454500	3.24425500	-0.76046400	H -3.12466100	-3.56682600	0.50219600
H -2.37190800	-4.18084600	0.79084600	C -4.95425100	-0.42139800	-0.77125900
H -2.36790000	4.18241400	0.79135300	H -3.20866100	-0.00960500	-1.90613400
Fe -1.09740800	0.00023500	0.09508400	C -5.60092500	-1.28245000	0.12594000
C -0.62674300	0.00001200	1.73924900	H -5.41135100	-3.10315100	1.25839200
H -2.57207400	0.00101200	0.47278600	H -5.47879500	0.45294100	-1.13903500
C 6.54066000	-0.00188800	1.03892300	C 2.23782800	1.10112300	-1.20370300
H 6.44161800	-0.00248000	2.12230900	H 1.97091700	0.95609400	1.11255900
C 7.76922200	-0.00159400	0.52167200	Fe 1.19974800	0.36097500	-0.05793900
H 7.95777900	-0.00107100	-0.54615700	C -6.92346400	-1.00686600	0.56818100
H 8.64099700	-0.00189300	1.16470900	N -7.99711600	-0.77947900	0.93175800
Fe + CN-Ph-CHCH2-interm (CN bond)			Fe + CN-Ph-CHCH2-interm (C=C bond)		
P 1.23998400	2.21561600	0.06325600	P -0.23820100	2.06934900	0.10555600
P 1.23865500	-2.21604000	0.06329200	P 2.54164500	-1.39184800	0.16410000
C 1.54779100	2.44685700	1.88145900	C -1.55193900	1.34557500	1.20145800
C 1.54661400	-2.44740100	1.88144600	C 1.58044900	-2.46347100	1.34438500
H 0.56420400	2.53367500	2.35123600	H -2.30636800	0.90399500	0.54395200
H 0.56304300	-2.53363300	2.35136800	H 1.01254700	-3.17350700	0.73771900
H 2.11175900	3.35278400	2.11210700	H -2.05325800	2.09219000	1.82047700
H 2.11010600	-3.35362600	2.11207700	H 2.22214100	-3.04174400	2.01269400
C 2.24346000	1.20428400	2.40058600	C -0.91974000	0.26532500	2.05451100
C 2.24302500	-1.20517900	2.40041900	C 0.63225100	-1.57795400	2.12901100

H	2.24386000	1.20203100	3.49909300	H	-1.69587000	-0.33607100	2.54284900
H	2.24370100	-1.20294700	3.49892700	H	-0.11431400	-2.18714300	2.65449100
H	3.28470900	1.17406100	2.07070400	H	-0.30022200	0.70794100	2.83710900
H	3.28420500	-1.17544100	2.07027400	H	1.17908400	-1.00621700	2.88113900
N	1.56135200	-0.00029000	1.89723000	N	-0.04377800	-0.60794500	1.24099300
C	-0.27360600	-3.30354700	-0.19451300	C	2.86570600	-2.60947700	-1.23614800
C	-0.27161300	3.30399000	-0.19480800	C	-1.25969900	2.68376900	-1.34849100
H	-1.02504500	-2.76452900	0.39345200	H	1.85298100	-2.98577900	-1.42013800
H	-1.02335100	2.76559200	0.39334400	H	-1.65757300	1.74149700	-1.73989700
C	2.64062600	-3.10608700	-0.81724100	C	4.20047000	-1.12709500	1.00145500
C	2.64265200	3.10481600	-0.81701000	C	0.37386200	3.62129000	0.96956400
C	3.99276200	-2.85334200	-0.15476000	C	4.04544600	-0.66446600	2.44800700
C	3.99442500	2.85158800	-0.15396900	C	0.55402500	3.41929500	2.47197500
O	0.41164600	0.00004100	-2.88490800	O	2.84515700	1.65675500	-2.04304000
H	2.41409600	4.17361300	-0.74207100	H	-0.40825600	4.37192600	0.81396800
H	2.41160300	-4.17476000	-0.74196800	H	4.68431700	-2.10923200	1.00588600
C	2.70800300	2.70848900	-2.29108100	C	1.67786700	4.12298800	0.35146500
C	2.70561300	-2.71018400	-2.29144300	C	5.07177800	-0.14521400	0.22147900
H	1.76934000	2.87209300	-2.82034000	H	1.60661400	4.28803800	-0.72353000
H	1.76668700	-2.87355000	-2.82031200	H	5.23688600	-0.45198800	-0.81178500
H	2.96289200	1.65149100	-2.38692700	H	2.48094700	3.40429200	0.52462200
H	2.96089700	-1.65331600	-2.38765900	H	4.61816100	0.84737300	0.20686400
H	3.48296100	3.29237300	-2.79701600	H	1.96513700	5.07100300	0.81574900
H	3.48014400	-3.29452800	-2.79749700	H	6.05120100	-0.05944600	0.70099100
C	-0.75514800	-3.34512700	-1.64275300	C	3.34531500	-1.95345800	-2.52814800
C	-0.75322100	3.34544500	-1.64303000	C	-0.43195600	3.33366300	-2.45452900
H	-0.09347400	-3.95082100	-2.26684800	H	4.36442800	-1.57164100	-2.44154200
H	-0.09125500	3.95060600	-2.26732900	H	-0.06626500	4.31894900	-2.15655300
H	-0.82785000	-2.35234300	-2.08674900	H	2.70174600	-1.12642500	-2.82833500
H	-0.82648700	2.35257700	-2.08674700	H	0.42442500	2.72643700	-2.74810600
H	-1.74779100	-3.80210600	-1.68686000	H	3.34449800	-2.69031500	-3.33664600
H	-1.74561600	3.80295400	-1.68720500	H	-1.05661200	3.47946800	-3.34044500
C	-0.13983100	-4.71578000	0.37255000	C	3.74465800	-3.79694600	-0.84939500
C	-0.13697400	4.71630600	0.37184200	C	-2.43935700	3.56987900	-0.95267400
H	0.13513900	-4.72215400	1.42852700	H	3.41659400	-4.28117600	0.07323700
H	0.13811400	4.72282900	1.42778700	H	-3.08876600	3.10156300	-0.21162800
H	0.60075100	-5.30463200	-0.17535800	H	4.78909900	-3.50111100	-0.72536400
H	0.60388200	5.30458300	-0.17631700	H	-2.10798900	4.53342700	-0.55732200
H	-1.09607700	-5.23979800	0.28183400	H	3.71681100	-4.55088900	-1.64149700
H	-1.09293600	5.24083500	0.28108000	H	-3.05147200	3.78054200	-1.83451400
H	-0.54854200	0.00065000	0.55700200	H	0.04909600	-0.50997600	-1.30347600
H	0.57752700	-0.00014100	2.34638200	H	-0.67177100	-1.17056100	0.60374500
N	-1.02927300	0.00012300	2.67473900	C	-0.65094700	-1.32545200	-1.81054000
C	-1.39399600	0.00041800	1.51622200	H	5.03433900	-0.50341700	2.88690700
C	-2.72568700	0.00062100	0.87009600	H	3.49771300	0.27918200	2.49849700
C	-2.87440000	0.00075500	-0.51108200	H	3.53036300	-1.39799600	3.07126700
C	-4.13782400	0.00093700	-1.08391200	H	0.92675100	4.34388100	2.92216600
C	-5.29151200	0.00099300	-0.29491300	H	-0.37770000	3.16363200	2.97944700
C	-3.87410400	0.00067100	1.67172900	H	1.28769800	2.63475100	2.67267000
C	-5.12962100	0.00085400	1.09928500	H	0.07106200	-1.92450800	-2.36474600
H	-1.98646600	0.00070900	-1.13407100	C	-1.48530900	-2.09838500	-0.90302600
H	-4.23633200	0.00103400	-2.16505600	H	-1.10518600	-3.06270500	-0.57605400
H	-3.74848600	0.00055700	2.74845500	H	-1.19973500	-0.70987200	-2.52585300
H	-6.00157800	0.00089500	1.74357500	C	-2.84443500	-1.83712600	-0.61757900
H	4.77776600	-3.36867500	-0.71621600	C	-3.58929900	-2.71159600	0.22886200
H	4.77990200	3.36629400	-0.71533800	C	-3.56823100	-0.71893300	-1.12309300
H	4.22941600	-1.78649900	-0.15634800	C	-4.90050900	-2.48088000	0.55691500
H	4.23049400	1.78461500	-0.15508500	H	-3.09351000	-3.59390500	0.62268000
H	4.03519100	-3.21721500	0.87342200	C	-4.88651900	-0.48968300	-0.79750000
H	4.03669200	3.21582000	0.87409300	H	-3.08507700	-0.03758100	-1.81420000
Fe	1.08331300	-0.00016300	-0.08819200	C	-5.58457000	-1.35323400	0.06028600
C	0.66145700	-0.00007900	-1.75271500	H	-5.42551200	-3.17328000	1.20580500
H	2.52890800	-0.00066000	-0.46873100	H	-5.40203700	0.36893300	-1.21431900

C -6.60085100	0.00119300	-0.95138100	C -6.93386900	-1.10236900	0.40854400
H -6.55955100	0.00130900	-2.03878400	N -8.03571200	-0.89268800	0.69823500
C -7.80155900	0.00123300	-0.37159700	Fe 1.16453500	0.34347000	-0.10839100
H -7.93406600	0.00111200	0.70461300	C 2.15735900	1.12047600	-1.28368000
H -8.70539400	0.00138500	-0.96882500	H 1.95160100	0.99597900	0.96537400
Fe + CN-Ph-CHCH2-TS-H_N transfer (CN bond)			Fe + CN-Ph-CHCH2-TS-H_N transfer (C=C bond)		
P -1.26480700	-2.21765700	0.07191100	P -0.15657000	2.08989400	0.12738700
P -1.26473200	2.21768000	0.07190300	P 2.52270600	-1.44731000	0.13186500
C -1.42554700	-2.45081500	1.90631000	C -1.48751600	1.38979100	1.21269600
C -1.42554900	2.45086400	1.90629400	C 1.52746300	-2.51635900	1.28031900
H -0.40785700	-2.56406400	2.28946800	H -2.26215800	1.00100600	0.54647000
H -0.40788000	2.56413800	2.28949900	H 0.96178600	-3.20813800	0.65160600
H -1.98827800	-3.34566200	2.17977400	H -1.95450200	2.13757500	1.85679800
H -1.98830700	3.34570800	2.17971000	H 2.14929200	-3.11415500	1.95046200
C -2.04491200	-1.19242300	2.48266000	C -0.88861300	0.25485700	2.01944300
C -2.04492500	1.19247500	2.48264000	C 0.57794800	-1.62065400	2.05431200
H -1.91110600	-1.18096100	3.57439700	H -1.69281800	-0.35682500	2.45074600
H -1.91113600	1.18102000	3.57437900	H -0.22015900	-2.22736700	2.50613600
H -3.12405600	-1.17290600	2.29387000	H -0.30366900	0.65099900	2.85635400
H -3.12406600	1.17295700	2.29383200	H 1.10740400	-1.12998600	2.87765500
N -1.42275700	0.00002400	1.89228500	N -0.01314700	-0.58821500	1.18650100
C 0.20992700	3.32277900	-0.30897700	C 2.84541600	-2.64651900	-1.28561200
C 0.20980400	-3.32279900	-0.30902100	C -1.16155700	2.76784100	-1.31156900
H 1.00676700	2.80751600	0.23972200	H 1.82997300	-3.00909700	-1.48254800
H 1.00668800	-2.80753000	0.23960700	H -1.58794800	1.84641000	-1.72373400
C -2.74510800	3.07814400	-0.70037300	C 4.17400400	-1.21923400	0.99292800
C -2.74523300	-3.07808100	-0.70031700	C 0.51954900	3.59908600	1.01697200
C -4.03725100	2.78904400	0.06005500	C 4.00181300	-0.75581800	2.43750900
C -4.03733400	-2.78901600	0.06019600	C 0.70991200	3.34914500	2.51117800
O -0.57806100	-0.00000100	-2.91902300	O 2.86514100	1.58821200	-2.09566800
C -2.90800200	-2.68829600	-2.16854900	H -0.23799500	4.38004300	0.89106700
C -2.90779700	2.68843900	-2.16863400	H 4.63621500	-2.21175500	1.00463900
H -2.01436300	-2.87801900	-2.76304300	C 1.83243600	4.07204500	0.39498000
H -2.01409900	2.87811800	-2.76305400	C 5.08042600	-0.25658700	0.22934200
H -3.14330100	-1.62592000	-2.25428300	H 1.75360600	4.26834300	-0.67419600
H -3.14317200	1.62608400	-2.25443500	H 5.26489000	-0.57284800	-0.79782700
H -3.73140500	-3.25577100	-2.61282700	H 2.61232900	3.32181400	0.53746700
H -3.73112400	3.25599700	-2.61294800	H 4.64473700	0.74369400	0.19773700
C 0.60071300	3.34667400	-1.78463400	H 2.15842100	4.99664500	0.88053900
C 0.60049700	-3.34675800	-1.78470200	H 6.04958600	-0.18483200	0.73164100
H -0.10857500	3.92958800	-2.37713700	C 3.34239200	-1.98241500	-2.56663300
H -0.10885000	-3.92966400	-2.37714000	C -0.32022300	3.41919600	-2.40642800
H 0.66415600	2.34794400	-2.21640600	H 4.36008500	-1.60071300	-2.46492000
H 0.66395500	-2.34804500	-2.21651200	H 0.07058600	4.38827400	-2.08799300
H 1.57992000	3.82082300	-1.89734400	H 2.70280300	-1.15376700	-2.86998800
H 1.57967800	-3.82095100	-1.89745600	H 0.52018600	2.79751200	-2.71498100
C 0.08880500	4.74234000	0.24260200	H 3.35188700	-2.71435800	-3.37969200
C 0.08869700	-4.74233900	0.24261600	H -0.94273800	3.60003900	-3.28749000
H -0.12951300	4.76206800	1.31151600	C 3.70739900	-3.84844300	-0.90519900
H -0.12963700	-4.76203000	1.31152700	C -2.31338900	3.67953400	-0.89197800
H -0.68813900	5.31238300	-0.27373700	H 3.36477400	-4.33910500	0.00867600
H -0.68822700	-5.31241600	-0.27371500	H -2.97267100	3.21546900	-0.15699100
H 1.03153100	5.27698100	0.09199100	H 4.75362300	-3.56517200	-0.76714200
H 1.03143500	-5.27697000	0.09204200	H -1.95112300	4.62367500	-0.47735100
H 0.65860900	-0.00006700	0.43994600	H 3.67958500	-4.59273000	-1.70647800
H -0.25658900	0.00004100	2.31761200	H -2.92260300	3.92813800	-1.76606200
N 1.07214100	0.00005300	2.51904700	H -0.03087300	-0.48234000	-1.41824800
C 1.44913100	-0.00000400	1.34609900	H -0.79160400	-1.22454500	0.43927700
C 2.81058800	-0.00002200	0.77200300	C -0.75191200	-1.31127700	-1.74992100
C 3.01306600	-0.00009500	-0.60410100	H 4.98532400	-0.61749300	2.89602200
C 4.29763300	-0.00011400	-1.12751900	H 3.47331200	0.19898800	2.48059100
C 5.41923100	-0.00006500	-0.29329900	H 3.45702800	-1.47853000	3.04760000

C 3.92682700	0.00004400	1.61705400	H 1.12481800	4.24541300	2.98147100
C 5.20348400	0.00003200	1.09378900	H -0.22509300	3.11529800	3.02271700
H 2.15277900	-0.00013400	-1.26585700	H 1.41243400	2.52981700	2.68149800
H 4.43891900	-0.00018000	-2.20385200	H -0.11402100	-2.01794800	-2.28152000
H 3.75879100	0.00011100	2.68804500	C -1.50950400	-1.92912500	-0.62758700
H 6.05023600	0.00012300	1.77081700	H -1.22286900	-2.95852400	-0.41142200
H -4.87513300	3.28422700	-0.43978700	H -1.37351500	-0.81043700	-2.49547000
H -4.87523000	-3.28424400	-0.43957700	C -2.92819100	-1.71322600	-0.46448400
H -4.24526900	1.71647600	0.07455700	C -3.68813200	-2.57777600	0.36158800
H -4.24539500	-1.71645600	0.07468800	C -3.63750200	-0.63911700	-1.04932900
H -4.01101600	3.15004100	1.08960000	C -5.02745400	-2.37971200	0.60088800
H -4.01101400	-3.14998800	1.08974700	H -3.19107100	-3.42862000	0.81752400
H -2.53657700	4.15158300	-0.63476500	C -4.98301800	-0.43424500	-0.81597400
H -2.53669900	-4.15152400	-0.63477700	H -3.12541300	0.04071800	-1.72071300
H -2.54678100	0.00003800	-0.41106800	C -5.70487000	-1.29389600	0.01999200
C -0.76350800	0.00000200	-1.77454600	H -5.57343400	-3.06628800	1.23802200
Fe -1.10387200	0.00000900	-0.08750000	H -5.49360400	0.39733600	-1.28886200
C 6.75332800	-0.00008000	-0.89790800	C -7.08607800	-1.07857000	0.26734000
H 6.75510400	-0.00008200	-1.98607100	N -8.21079700	-0.90019100	0.47205900
C 7.93008700	-0.00012600	-0.27099600	Fe 1.18701000	0.32205000	-0.12250700
H 8.85684500	-0.00013600	-0.83197800	C 2.17360900	1.06726800	-1.32804800
H 8.02002200	-0.00016800	0.80959500	H 2.03091600	0.96471700	0.89237900
2Mo-cis + PhCHO-TS-H_M transfer			2Mo-trans + PhCHO-TS-H_M transfer		
O 2.25034100	3.18927900	-0.25458200	O 2.08784500	3.09518100	-0.79207700
P -1.52967400	1.68660700	0.14934400	P -1.56381600	1.65256700	0.18301800
P 2.60824900	-0.90799700	0.14817400	P 2.62811400	-0.85725200	0.16591400
C -1.69477600	1.40319100	1.98925100	C -1.72859400	1.35939400	2.02497800
C 2.56598500	-1.04732400	2.01286400	C 2.60968800	-0.98874000	2.03401900
H -2.22160300	0.45110600	2.10351800	H -2.25780300	0.40821000	2.13785300
H 2.02378700	-1.96862900	2.24231400	H 2.11160500	-1.93183300	2.27400500
H -2.30103800	2.17208400	2.47321400	H -2.33255400	2.12757800	2.51388200
H 3.56699100	-1.13436600	2.44019900	H 3.61743200	-1.02498200	2.45344800
C -0.33030300	1.30232100	2.65661600	C -0.36312400	1.25870900	2.68884000
C 1.81980400	0.12656900	2.63138300	C 1.81711400	0.15635200	2.64729600
H -0.45625800	1.04571200	3.71778200	H -0.48572600	0.97577100	3.74394500
H 1.69392200	-0.04582200	3.70946300	H 1.69351100	-0.01990100	3.72526700
H 0.19666800	2.25831200	2.61192400	H 0.14939200	2.22296100	2.66744900
H 2.37804900	1.05784300	2.50861700	H 2.34058100	1.10777500	2.52625400
N 0.50309800	0.28873700	1.98741300	N 0.49641000	0.27977400	1.99982000
C 2.61053700	-2.72572100	-0.34420700	C 2.72356700	-2.67954000	-0.29869400
C -3.13157300	0.95201000	-0.49358400	C -3.18826900	0.94662000	-0.44019000
H 1.75279600	-3.09305100	0.22848900	H 1.87822100	-3.08153300	0.26986600
H -3.02385800	-0.08858700	-0.17356800	H -3.08928800	-0.10095400	-0.13922700
C 4.34764800	-0.31152500	-0.25578000	C 4.32354800	-0.15125500	-0.23436200
C -1.73019100	3.54409900	-0.08950900	C -1.72308100	3.51551200	-0.02030300
C 4.80781300	0.83170100	0.64541800	C 4.65769100	1.06917800	0.62082700
C -0.99098600	4.36550200	0.96410900	C -0.87323300	4.28794700	0.98639300
O 0.59221300	0.46607400	-3.30364000	O 0.29579400	0.05983400	-3.36636900
H -2.80198800	3.74345900	0.01343300	H -2.77642500	3.74648600	0.17217700
H 5.00596300	-1.16765500	-0.07788400	H 5.03997600	-0.94315600	0.00749700
C -1.28297400	3.95329000	-1.49281800	C -1.37322000	3.94130600	-1.44645100
C 4.44147400	0.09130100	-1.72648900	C 4.43435500	0.18483700	-1.72039500
H -1.81499800	3.41598000	-2.27797800	H -1.97467100	3.43096800	-2.19826900
H 4.18839300	-0.72634600	-2.40266300	H 4.26451200	-0.68221900	-2.35988300
H -0.21671300	3.76633000	-1.62996000	H -0.32377700	3.74213400	-1.66648100
H 3.76609000	0.92099200	-1.94478900	H 3.71094900	0.95249800	-2.00018500
H -1.45992000	5.02291300	-1.64149400	H -1.54160300	5.01674100	-1.55989400
H 5.46054600	0.41300900	-1.96138300	H 5.43568500	0.56751000	-1.93986700
C 2.29932800	-2.92901300	-1.82460900	C 2.45426300	-2.93428200	-1.77885400
C -3.20168400	0.95486300	-2.01874900	C -3.30654100	0.97499900	-1.96187700
H 3.14502000	-2.65291500	-2.45832600	H 3.29636800	-2.62774600	-2.40300800
H -3.40136200	1.95413400	-2.41313300	H -3.52636700	1.97930200	-2.33145200

H 1.43753600	-2.33655200	-2.13662400	H 1.56929000	-2.39933300	-2.12559500
H -2.27819300	0.58602800	-2.46768200	H -2.39698200	0.62147600	-2.44842500
H 2.08116600	-3.98336700	-2.02000300	H 2.29839700	-4.00369400	-1.95020500
H -4.01873700	0.30765200	-2.34923100	H -4.12986000	0.32766800	-2.27601900
C 3.83699600	-3.52175300	0.09351300	C 3.98598200	-3.39484100	0.17621200
C -4.40319300	1.52379400	0.12684800	C -4.43469500	1.52629100	0.22375400
H 4.07601800	-3.37679400	1.14972000	H 4.19083900	-3.22584400	1.23573800
H -4.38513800	1.50258400	1.21860200	H -4.39363900	1.47776700	1.31371200
H 4.72038200	-3.26081700	-0.49424700	H 4.86477800	-3.08478000	-0.39442500
H -4.58509300	2.55405700	-0.19006200	H -4.60208800	2.56741700	-0.06434700
H 3.65750800	-4.59069500	-0.05704700	H 3.87537100	-4.47401400	0.03326600
H -5.26520600	0.93245200	-0.19549400	H -5.31512700	0.96007600	-0.09382400
H -0.49809300	-1.01601000	-0.12777400	H -0.49376100	-1.02838200	-0.20407900
H 0.02016600	-0.62116500	2.07722100	H 0.04599000	-0.64894000	2.07219000
C -0.95690400	-2.47653900	0.80024800	C -0.85205900	-2.49328900	0.67491000
C -2.36847300	-2.59683600	0.33088600	C -2.28618300	-2.61826900	0.27287800
C -2.64703600	-2.89813400	-1.00166200	C -2.63016400	-2.87754700	-1.05307500
C -3.95529400	-3.09259000	-1.41723200	C -3.95618800	-3.07377300	-1.40760500
C -4.99800100	-2.99486700	-0.50009000	C -4.95138600	-3.01887000	-0.43585500
C -3.41471900	-2.51000100	1.24736500	C -3.28459000	-2.57531700	1.24385600
C -4.72520100	-2.70563300	0.83222700	C -4.61290300	-2.77171500	0.88985000
H -1.83016900	-2.96228300	-1.71373400	H -1.85121100	-2.90973800	-1.80861000
H -4.16581200	-3.32249500	-2.45588100	H -4.21717100	-3.27181900	-2.44135600
H -6.02111700	-3.15233000	-0.82360500	H -5.98816500	-3.17743100	-0.71180500
H -3.17653900	-2.31027100	2.28602800	H -2.99469900	-2.40936600	2.27529900
H -5.53579100	-2.64428400	1.55031800	H -5.38588500	-2.74428900	1.65029400
H 5.82785700	1.11831200	0.37199200	H 5.65491600	1.43304600	0.35544900
H 4.18056200	1.71585100	0.52912200	H 3.95626700	1.88599100	0.44781500
H 4.82409800	0.55416700	1.70122400	H 4.67216800	0.84086100	1.68836000
H -1.14907600	5.43074100	0.77032100	H -0.99209200	5.36163200	0.81252800
H -1.34412300	4.16643300	1.97782000	H -1.16690000	4.09418600	2.01993100
H 0.08520300	4.18806700	0.92801300	H 0.18761200	4.05693000	0.87290700
O -0.67537700	-2.26706800	1.99118300	O -0.51627500	-2.34394900	1.86310100
H -0.23945100	-2.97649500	0.13304600	H -0.16513800	-2.96471500	-0.04478400
N 0.60422200	0.49841700	-2.12528600	Mo 0.60264400	0.53600400	-0.28415700
C 1.66046700	2.18835500	-0.25087500	C 0.41966200	0.25545500	-2.23203300
Mo 0.60671000	0.50702000	-0.31385500	N 1.52684500	2.08084300	-0.53821100
2Mo-<i>cis</i> + PhCHO-interm			2Mo-<i>trans</i> + PhCHO-interm		
O 2.23101700	3.07763800	-0.12373500	O 2.08524500	3.05383900	-0.78017800
P -1.55580700	1.68528600	0.16730200	P -1.58348900	1.65356600	0.18940500
P 2.60269400	-0.94958700	0.13912200	P 2.64136100	-0.86909900	0.17536200
C -1.69465400	1.41060800	2.00381500	C -1.76714300	1.29226400	2.01051400
C 2.50168200	-1.13177200	1.99024600	C 2.58230700	-1.03085600	2.03330400
H -2.22033200	0.45835600	2.12249800	H -2.28939400	0.33301200	2.07637800
H 1.90447700	-2.03060400	2.16913900	H 2.07310200	-1.97597700	2.23844500
H -2.28743300	2.18444800	2.49577900	H -2.38212300	2.03897800	2.51842900
H 3.48237300	-1.27740500	2.44713300	H 3.58046500	-1.07378400	2.47419900
C -0.31879700	1.28645500	2.64263100	C -0.40929800	1.16436700	2.68425900
C 1.77688800	0.05296200	2.61436200	C 1.76613700	0.09916300	2.64299400
H -0.43843000	0.99548800	3.69574500	H -0.55204400	0.79844800	3.71092400
H 1.60502300	-0.15703400	3.67940500	H 1.59383500	-0.11975500	3.70637700
H 0.20734400	2.24617900	2.63162500	H 0.08207300	2.13906400	2.75630500
H 2.38350400	0.96241100	2.55865900	H 2.30525800	1.05007300	2.59160900
N 0.48795500	0.27769100	1.93976700	N 0.47238400	0.24275500	1.94935200
C 2.63724100	-2.74362500	-0.42027200	C 2.73413000	-2.67803000	-0.33073300
C -3.17584200	0.98148700	-0.46228900	C -3.20034100	0.98077500	-0.48718800
H 1.67978400	-3.10798500	-0.03391300	H 1.85399000	-3.07980500	0.18274500
H -3.08533000	-0.07183200	-0.17843500	H -3.12342900	-0.07704000	-0.21451200
C 4.32558200	-0.30356500	-0.25442900	C 4.32871600	-0.13862100	-0.20351200
C -1.70008900	3.53934200	-0.11838500	C -1.70489300	3.52145400	0.03303400
C 4.82751900	0.72547300	0.75587900	C 4.65026900	1.06084800	0.68590700
C -0.99542500	4.37194600	0.94997300	C -0.84819800	4.25049400	1.06589000

O 0.73254000	0.76673200	-3.28316300	O 0.31721800	0.06063500	-3.37772900
H -2.77262400	3.75328300	-0.06371000	H -2.75558500	3.75840500	0.23230200
H 4.98090800	-1.17888600	-0.20109700	H 5.04670300	-0.93353500	0.02380300
C -1.19532900	3.91461200	-1.51161400	C -1.35209900	3.98627400	-1.37991000
C 4.37894600	0.26384400	-1.67268800	C 4.45063700	0.23358100	-1.68016800
H -1.67916300	3.34347700	-2.30397400	H -1.95839100	3.50429000	-2.14626400
H 5.40763800	0.54184400	-1.92097200	H 4.27658800	-0.61481000	-2.34261900
H -0.12031300	3.74904800	-1.59524800	H -0.30420400	3.78889200	-1.60817700
H 4.03525800	-0.44636200	-2.42517700	H 3.73880600	1.01653100	-1.94641000
H -1.38626700	4.97545200	-1.69980800	H -1.51317700	5.06567100	-1.45965900
H 3.76048400	1.15855200	-1.75850000	H 5.45716800	0.61149700	-1.88292400
C 2.60889800	-2.88248100	-1.94040100	C 2.54602300	-2.90338800	-1.82799800
C -3.28393100	1.04161500	-1.98399300	C -3.29862800	1.05467400	-2.00867100
H 3.57230700	-2.62375200	-2.38618400	H 3.42843200	-2.60423400	-2.39775800
H -3.48106000	2.05750400	-2.33545900	H -3.51819200	2.06850700	-2.35115700
H 1.84347600	-2.24970500	-2.39387800	H 1.69028400	-2.35216000	-2.21932700
H -2.37736400	0.67977900	-2.47274000	H -2.38320100	0.71901300	-2.49722300
H 2.39540500	-3.91951600	-2.21483300	H 2.38134100	-3.96699000	-2.02322200
H -4.11573100	0.41516900	-2.31651300	H -4.11500900	0.41327200	-2.35096100
C 3.74699500	-3.58738400	0.20178900	C 3.96308400	-3.41353300	0.19858500
C -4.42228900	1.55008200	0.21085900	C -4.44886600	1.55455000	0.17860900
H 3.75817200	-3.52560700	1.29162300	H 4.10510800	-3.27444800	1.27227200
H -4.38310400	1.47165900	1.29889900	H -4.42310400	1.46860300	1.26639500
H 4.73473900	-3.29921200	-0.16671600	H 4.87597900	-3.09596200	-0.31142300
H -4.58793800	2.59861600	-0.05067100	H -4.60088300	2.60613500	-0.07851400
H 3.60147600	-4.63878900	-0.06375500	H 3.85325300	-4.48737700	0.02078700
H -5.30170100	0.99225000	-0.12322200	H -5.32964000	1.00741600	-0.16911300
H -0.66365600	-1.23507800	-0.03743900	H -0.62737400	-1.19509100	-0.08374300
H -0.06913900	-0.69904700	2.01792700	H 0.00810600	-0.76925500	1.97933300
C -0.93708400	-2.17441100	0.65332700	C -0.82347700	-2.21272400	0.53423100
C -2.36094600	-2.51104100	0.23124500	C -2.27783000	-2.52476000	0.20591700
C -2.67728900	-2.77518100	-1.10076100	C -2.69260600	-2.74097000	-1.10754100
C -3.97009000	-3.12508300	-1.46388100	C -4.01383200	-3.06088100	-1.38722100
C -4.96457000	-3.22033800	-0.49414200	C -4.93772700	-3.17336300	-0.35188700
C -3.35576500	-2.61620200	1.19659100	C -3.20208100	-2.64984700	1.23692400
C -4.65274100	-2.96717500	0.83553000	C -4.52715200	-2.97006100	0.95959200
H -1.90367200	-2.70020700	-1.86062000	H -1.97414300	-2.65538100	-1.91849200
H -4.20492000	-3.32711200	-2.50366200	H -4.32510600	-3.22792100	-2.41300700
H -5.97455300	-3.49787300	-0.77580600	H -5.96945400	-3.42834400	-0.56852400
H -3.07897900	-2.43131700	2.22835300	H -2.84735000	-2.51085300	2.25204100
H -5.42094600	-3.05168200	1.59727600	H -5.23966600	-3.07145200	1.77173200
H 5.83791700	1.04010200	0.47808700	H 5.64866600	1.43434300	0.43952800
H 4.20263100	1.61957400	0.76538900	H 3.94851000	1.88041500	0.52667600
H 4.87986800	0.32775400	1.77075000	H 4.65329100	0.80578600	1.74707700
H -1.13989700	5.43459200	0.73315000	H -0.95227400	5.33027200	0.92389300
H -1.38748500	4.18952500	1.95199600	H -1.14920700	4.02801700	2.09106300
H 0.08012600	4.18828900	0.95861500	H 0.21015900	4.00891800	0.95144200
O -0.74089600	-1.94408500	1.94300000	O -0.51202300	-2.10923000	1.81343200
H -0.28094200	-2.95039300	0.20891400	H -0.19828800	-2.91322000	-0.05519800
Mo 0.57774000	0.46211800	-0.30682800	Mo 0.60087000	0.52620400	-0.28260900
N 0.65028900	0.61099400	-2.12072500	N 1.50531700	2.04277300	-0.57036100
C 1.61620600	2.09458700	-0.18844600	C 0.42421100	0.23918900	-2.24069900
2Mo-cis + PhCHO-TS-H_N transfer			2Mo-trans + PhCHO-TS-H_N transfer		
O 2.24721900	3.11085800	-0.49686200	O 2.15290900	3.00617400	-0.82983300
P -1.53662100	1.71042300	0.16774000	P -1.54393100	1.69300100	0.18615500
P 2.63127700	-0.91813300	0.16538300	P 2.63485300	-0.90835100	0.17590200
C -1.73109600	1.35953400	1.98532600	C -1.74709900	1.33131500	2.00325000
C 2.50953700	-1.13419000	2.01099000	C 2.52931100	-1.12671100	2.02436100
H -2.27371400	0.41208600	2.05161300	H -2.30431800	0.39186900	2.06396600
H 1.94609600	-2.05720400	2.17135700	H 1.99566800	-2.06591600	2.19162600
H -2.32774700	2.12235300	2.49070800	H -2.33480700	2.09923700	2.51192000
H 3.49039500	-1.24695700	2.47756600	H 3.51624000	-1.20777300	2.48523600

C -0.37528800	1.19404700	2.65584000	C -0.39511800	1.14757700	2.67597200
C 1.73309800	0.01587600	2.63636300	C 1.72527800	0.00458900	2.64834200
H -0.52959400	0.83375400	3.68318300	H -0.55631100	0.75960300	3.69249700
H 1.52477100	-0.22998700	3.68759700	H 1.51233300	-0.25215600	3.69639900
H 0.14247800	2.15643800	2.73015100	H 0.11908500	2.10899100	2.78154500
H 2.32487800	0.93769800	2.63464400	H 2.30157900	0.93630900	2.65899400
N 0.46534500	0.23720100	1.92037200	N 0.46048800	0.21726500	1.92410500
C 2.65243700	-2.70631600	-0.41720100	C 2.72022300	-2.70054400	-0.39036600
C -3.13667000	1.02403200	-0.53296900	C -3.17064300	1.05547000	-0.50308200
H 1.73349900	-3.08285700	0.04449500	H 1.80882800	-3.10388500	0.06455300
H -3.07283500	-0.02404700	-0.22223300	H -3.12456100	-0.00069200	-0.21628800
C 4.36561600	-0.27146000	-0.15846700	C 4.33773300	-0.18498100	-0.14037700
C -1.67504400	3.57639200	-0.00937300	C -1.61951800	3.56323800	0.03714700
C 4.75941300	0.84895700	0.80154400	C 4.64025300	0.99134600	0.78591300
C -0.86702200	4.32747100	1.04636400	C -0.72858900	4.26114600	1.06268100
O 0.50017900	0.30497800	-3.28615100	O 0.29990900	0.00600300	-3.36497400
H -2.73476600	3.80283600	0.14858000	H -2.66054100	3.82649700	0.25359200
H 5.03151000	-1.12172700	0.02138200	H 5.04272100	-0.99073500	0.09008900
C -1.27700300	4.02866200	-1.41381000	C -1.27512900	4.02708900	-1.37792600
C 4.51882400	0.18018600	-1.60994100	C 4.50746700	0.22033500	-1.60365100
H -1.86434700	3.54554900	-2.19447000	H -1.91312200	3.57496000	-2.13675800
H 4.30384000	-0.61609000	-2.32305300	H 4.34488300	-0.60994800	-2.29116600
H -0.22499700	3.81656700	-1.61010800	H -0.23960000	3.79327300	-1.62734000
H 3.85059100	1.01390400	-1.83263000	H 3.81367800	1.01808500	-1.87268700
H -1.42340400	5.10882100	-1.50829800	H -1.39746100	5.11234600	-1.44586900
H 5.54490000	0.51592000	-1.78697900	H 5.52384300	0.59121400	-1.76646600
C 2.50164400	-2.85131800	-1.92940100	C 2.60022500	-2.87475400	-1.90162000
C -3.18254000	1.04555000	-2.05889900	C -3.25348400	1.11180900	-2.02612900
H 3.42002100	-2.58302900	-2.45601200	H 3.51967500	-2.58842500	-2.41657900
H -3.36943300	2.05027800	-2.44483400	H -3.44437300	2.12606800	-2.38382800
H 1.69429500	-2.23147700	-2.32195900	H 1.78302000	-2.28565100	-2.31877400
H -2.25766300	0.67560500	-2.50359200	H -2.34241600	0.74755600	-2.50180700
H 2.28011400	-3.89277300	-2.18018200	H 2.41381500	-3.92645800	-2.13764200
H -3.99947700	0.40790900	-2.40702400	H -4.08263900	0.48668700	-2.36802900
C 3.81927200	-3.53437200	0.11499500	C 3.90893600	-3.47749400	0.17083800
C -4.40304500	1.62261100	0.07388200	C -4.40971900	1.66967400	0.14417000
H 3.93252700	-3.45140800	1.19797000	H 3.99797100	-3.38313400	1.25490600
H -4.40263700	1.58747900	1.16510900	H -4.39345600	1.60048900	1.23339300
H 4.76541000	-3.24779700	-0.35071200	H 4.85105400	-3.15473700	-0.27917900
H -4.55238000	2.66038800	-0.23535500	H -4.53288800	2.72054400	-0.13053500
H 3.65604800	-4.59120900	-0.11625400	H 3.79329200	-4.54149700	-0.05590300
H -5.27331400	1.05593800	-0.26907700	H -5.30161500	1.13958100	-0.20172000
H -0.67022800	-1.24332800	-0.05123100	H -0.66808900	-1.24005000	-0.08084000
H -0.09247100	-0.80333800	1.97014600	H -0.08495500	-0.85000300	1.95088100
C -0.93149500	-2.18089600	0.61283400	C -0.91312000	-2.19549400	0.56477100
C -2.37345100	-2.49912000	0.24812400	C -2.36193400	-2.50460200	0.22242500
C -2.74147900	-2.76059100	-1.07144900	C -2.75402400	-2.74760100	-1.09371100
C -4.05272500	-3.08650100	-1.38801500	C -4.07267000	-3.06128100	-1.39138000
C -5.01447800	-3.16041600	-0.38425700	C -5.01729500	-3.14166000	-0.37209200
C -3.33636100	-2.58322100	1.24754400	C -3.30774300	-2.59545800	1.23749700
C -4.65149000	-2.91032900	0.93287400	C -4.63007200	-2.91057600	0.94162300
H -1.99414900	-2.70434700	-1.85851500	H -2.02041900	-2.68710100	-1.89316500
H -4.32695400	-3.28708900	-2.41834700	H -4.36572500	-3.24753500	-2.41916400
H -6.03867300	-3.41957800	-0.62965000	H -6.04720500	-3.39135400	-0.60285300
H -3.02189800	-2.40323200	2.26920300	H -2.97508300	-2.43101300	2.25597000
H -5.39378600	-2.97873000	1.72141200	H -5.35894700	-2.98465800	1.74202800
H 5.78118900	1.17142300	0.58027500	H 5.64480500	1.36878600	0.57300400
H 4.11366700	1.72093800	0.69109000	H 3.94310600	1.81566100	0.62988700
H 4.73840700	0.53257400	1.84579200	H 4.61613700	0.70982800	1.83999500
H -0.99075700	5.40440600	0.89844700	H -0.80323900	5.34432700	0.92827500
H -1.19222900	4.09997900	2.06295500	H -1.02252400	4.04037200	2.09015300
H 0.19951100	4.11049700	0.96621700	H 0.32058200	3.98906700	0.93378100
O -0.68669000	-1.97375700	1.91029400	O -0.64056100	-2.02053900	1.86204600

H -0.30111100 -2.96223800 0.14572900	H -0.28746600 -2.95868000 0.06327800
Mo 0.60357900 0.48910800 -0.29740900	Mo 0.62084300 0.52153900 -0.27938300
N 0.55071400 0.39743000 -2.11465400	N 1.54803300 2.01192100 -0.60902000
C 1.63704200 2.12694000 -0.40940300	C 0.42048300 0.20227800 -2.23192800
2Mo-cis + PhCOCH₃-TS	2Mo-trans + PhCOCH₃-TS
O 2.16138500 3.15674100 -0.38927300	O 2.05143700 2.94230100 -1.11251800
P -1.53889300 1.69107100 0.18720400	P -1.52085900 1.71537200 0.20078400
P 2.70622000 -0.78871100 0.08751400	P 2.71922900 -0.77904300 0.13547600
C -1.60751000 1.50796500 2.04227600	C -1.57918000 1.58685000 2.06349200
C 2.63409400 -1.00417300 1.94291000	C 2.67673900 -0.94455600 2.00071400
H -2.13045400 0.56551100 2.23007400	H -2.12620000 0.66617700 2.28718500
H 2.09635600 -1.93856800 2.12525500	H 2.17865200 -1.89187800 2.22518200
H -2.17513500 2.30972800 2.51893400	H -2.11863900 2.42002800 2.51984400
H 3.62619000 -1.11035300 2.38714900	H 3.68004200 -0.99775700 2.43114200
C -0.21089300 1.41131400 2.63945800	C -0.17948000 1.47426100 2.64922600
C 1.87753500 0.14095400 2.60366400	C 1.89515600 0.19828400 2.63609400
H -0.28736600 1.21503800 3.71791300	H -0.25117300 1.28965600 3.73031800
H 1.76571100 -0.06610300 3.67701800	H 1.77193800 0.00220900 3.71046100
H 0.33959400 2.34680800 2.51382000	H 0.38263700 2.40056300 2.51105100
H 2.43418600 1.07637600 2.50866200	H 2.44275900 1.13824400 2.53854900
N 0.55368600 0.33199900 1.98608900	N 0.57588100 0.38235700 2.00376000
C 2.94256300 -2.55449200 -0.51337200	C 3.02719200 -2.56130900 -0.39164400
C -3.21435600 1.03499700 -0.33883400	C -3.22610200 1.09438100 -0.27332600
H 1.99780200 -3.00873200 -0.21216700	H 2.21067400 -3.07484100 0.11975100
H -3.13092600 -0.02086600 -0.07208600	H -3.17197500 0.05147600 0.04920100
C 4.38467900 0.00178200 -0.25933000	C 4.35730800 0.08593600 -0.19826800
C -1.67975600 3.54162400 -0.15545300	C -1.58119700 3.56336100 -0.15580400
C 4.79293500 1.05084200 0.77241900	C 4.57313600 1.31714500 0.67934100
C -0.94462500 4.41400700 0.85930400	C -0.65979200 4.37577600 0.75148500
O 0.43027200 0.30033800 -3.29883300	O 0.07144900 -0.27543200 -3.29273900
H -2.74933000 3.76269400 -0.07565300	H -2.61384600 3.85952500 0.05885800
H 5.10545400 -0.82081300 -0.20489800	H 5.12645500 -0.64775400 0.06417200
C -1.22111600 3.87179900 -1.57614700	C -1.28008700 3.86346800 -1.62475100
C 4.42845600 0.59441000 -1.66826600	C 4.50297600 0.44110000 -1.67754900
H -1.73145400 3.27620900 -2.33281600	H -1.91812900 3.30594400 -2.30920700
H 4.15683000 -0.12663800 -2.43897900	H 4.43283000 -0.43261100 -2.32576000
H -0.15039900 3.70219300 -1.69137800	H -0.24377200 3.63092200 -1.86879900
H 3.74940600 1.44254200 -1.75783200	H 3.73938600 1.15377200 -1.99023700
H -1.41856700 4.92657800 -1.79155000	H -1.43697200 4.92935800 -1.81814700
H 5.44007500 0.95052300 -1.88624300	H 5.48085600 0.90122000 -1.84944800
C 3.01948800 -2.63840200 -2.03655800	C 2.82587100 -2.78512300 -1.88852900
C -3.41073800 1.11546000 -1.85102200	C -3.46004600 1.09625800 -1.78224600
H 3.98576200 -2.29309500 -2.41129700	H 3.65362800 -2.38404200 -2.47670500
H -3.59638900 2.14100200 -2.18018800	H -3.65752400 2.10287800 -2.15824000
H 2.23497800 -2.05108800 -2.51741900	H 1.90474700 -2.32393700 -2.24605000
H -2.54688500 0.72973700 -2.39566400	H -2.61067600 0.68400100 -2.32875700
H 2.90550500 -3.67869900 -2.35565700	H 2.77397100 -3.85795000 -2.09739700
H -4.28067400 0.51951500 -2.13903800	H -4.33568700 0.48511900 -2.01549500
C 4.08093800 -3.32661000 0.14832800	C 4.34235800 -3.16355000 0.09646500
C -4.40553700 1.62699900 0.40968400	C -4.38131100 1.76485800 0.46598300
H 4.01800400 -3.31699600 1.23845700	H 4.50243100 -3.01457300 1.16683900
H -4.31259300 1.52501100 1.49255500	H -4.26801200 1.72239100 1.55077600
H 5.06127600 -2.93695500 -0.13715400	H 5.20120500 -2.74867200 -0.43646400
H -4.55364000 2.68546100 0.17896800	H -4.50039600 2.81232400 0.17630100
H 4.05013200 -4.37311000 -0.17071700	H 4.34430100 -4.24241300 -0.08668900
H -5.31853100 1.10330500 0.11137700	H -5.31667700 1.25517300 0.21670200
H -0.39177300 -1.20400700 0.01687100	H -0.41092000 -1.20376400 0.03023500
H 0.00522300 -0.53660200 2.13497800	H 0.02071900 -0.48161100 2.16502300
C -1.19545700 -2.34533800 1.05484500	C -1.18704400 -2.28848500 1.07842600
C -2.51149000 -2.40348800 0.31270100	C -2.50592200 -2.37558600 0.34075600
C -2.59829600 -2.60271800 -1.06493800	C -2.59654000 -2.61664000 -1.02973300
C -3.83253400 -2.76820100 -1.67498900	C -3.83206400 -2.80579600 -1.63088000

C -4.99825500	-2.74563400	-0.91446700	C -4.99530700	-2.76615100	-0.86787900
C -3.68256700	-2.37941200	1.06815100	C -3.67507500	-2.33514800	1.09872500
C -4.91999300	-2.54948500	0.45806900	C -4.91347900	-2.52925200	0.49817500
H -1.69469400	-2.58718700	-1.66400600	H -1.69631200	-2.62171900	-1.63374500
H -3.88804900	-2.90934000	-2.74890600	H -3.88959200	-2.97972000	-2.69983600
H -5.96239800	-2.87991100	-1.39267500	H -5.96024900	-2.91930800	-1.33873900
H -3.60199300	-2.23325600	2.13915600	H -3.59121100	-2.15745400	2.16467100
H -5.82393100	-2.53432900	1.05760800	H -5.81546100	-2.50145500	1.10023300
H 5.77857700	1.44850600	0.51219800	H 5.53760300	1.76994400	0.43010600
H 4.10049700	1.89355800	0.78581600	H 3.80708200	2.07501300	0.51297600
H 4.86703900	0.64294300	1.78225900	H 4.60043900	1.07040700	1.74246100
H -1.09342500	5.46799300	0.60523900	H -0.74199500	5.43601600	0.49363600
H -1.30963800	4.27342900	1.87842200	H -0.91934100	4.27939300	1.80741800
H 0.13055400	4.22991500	0.84521700	H 0.38538500	4.09126300	0.61878900
O -1.15978600	-1.84328300	2.19995000	O -1.16156900	-1.76981600	2.21880500
N 0.49661400	0.37415500	-2.12454500	Mo 0.58946400	0.45934600	-0.29017700
C 1.57316300	2.15485600	-0.34840200	C -0.28338400	-3.48081200	0.80882400
Mo 0.57809300	0.44927000	-0.31571400	H -0.80103900	-4.36749200	1.19168800
C -0.30079400	-3.53555500	0.75698600	H -0.07620800	-3.63787200	-0.24850400
H -0.81396900	-4.42183800	1.14758300	H 0.64429800	-3.37090900	1.36705500
H -0.12657200	-3.68846700	-0.30688200	C 0.27600400	0.01290200	-2.19070900
H 0.64316500	-3.43681700	1.28923400	N 1.47868900	1.97161500	-0.74027100
1W-cis + H₂-TS			1W-trans + H₂-TS		
W 0.15536000	0.10146400	0.00000000	W 0.16462300	-0.08039300	0.00000000
P -0.03661800	-0.36377800	-2.42667600	C 1.98916600	-0.84660600	0.00000000
P -0.03661800	-0.36377800	2.42667600	O 3.06878700	-1.27743000	0.00000000
N 1.58470600	1.22675500	0.00000000	N -0.54399600	-1.74231500	0.00000000
O 2.54112000	1.92887000	0.00000000	N -1.46091800	1.44572000	0.00000000
C -1.06410300	1.64724800	0.00000000	H 0.01690500	1.90627200	0.00000000
O -1.77741100	2.56536800	0.00000000	H 0.92300800	1.76528100	0.00000000
H 1.11367200	-1.60773200	0.00000000	P -0.08539900	0.36364200	-2.42397200
N -1.27655500	-1.61993900	0.00000000	P -0.08539900	0.36364200	-2.42397200
H 0.21167800	-1.86666100	0.00000000	C -2.25777800	1.61106900	-1.19883600
C -0.79761000	0.85111200	-3.63787800	C -2.25777800	1.61106900	1.19883600
C -0.79761000	0.85111200	3.63787800	C -0.72713900	-0.99670900	3.54295500
H -0.68423500	0.39739800	-4.62836800	C -0.72713900	-0.99670900	-3.54295500
H -0.68423500	0.39739800	4.62836800	H -0.70207500	-0.58243200	4.55697300
C -2.28689800	1.05480700	-3.36926800	H -0.70207500	-0.58243200	-4.55697300
C -2.28689800	1.05480700	3.36926800	C -2.17105200	-1.36334000	3.20532400
H -2.45922900	1.47703900	-2.37818600	C -2.17105200	-1.36334000	-3.20532400
H -2.45922900	1.47703900	2.37818600	H -2.25707300	-1.73738800	2.18369400
H -2.85904800	0.12907200	-3.45260500	H -2.25707300	-1.73738800	-2.18369400
H -2.85904800	0.12907200	3.45260500	H -2.85597300	-0.52211800	3.32462900
H -2.69416500	1.75815200	-4.10168000	H -2.85597300	-0.52211800	-3.32462900
H -2.69416500	1.75815200	4.10168000	H -2.50804700	-2.15850300	3.87692300
C -0.05755300	2.18694700	-3.60849000	H -2.50804700	-2.15850300	-3.87692300
C -0.05755300	2.18694700	3.60849000	C 0.16783000	-2.23380600	3.48260300
H -0.52416900	2.88400200	-4.31080000	C 0.16783000	-2.23380600	-3.48260300
H -0.52416900	2.88400200	4.31080000	H -0.20946500	-2.99129500	4.17624700
H 0.99270600	2.09224500	-3.88544500	H -0.20946500	-2.99129500	-4.17624700
H 0.99270600	2.09224500	3.88544500	H 1.20142200	-2.02087600	3.75485100
H -0.10028700	2.63331200	-2.61296700	H 1.20142200	-2.02087600	-3.75485100
H -0.10028700	2.63331200	2.61296700	H 0.16730000	-2.66646300	2.48130500
C 1.49397300	-1.05739600	-3.27507700	H 0.16730000	-2.66646300	-2.48130500
C 1.49397300	-1.05739600	3.27507700	C 1.30396500	1.22131100	3.36251400
H 1.69046500	-1.93223300	-2.64355200	C 1.30396500	1.22131100	-3.36251400
H 1.69046500	-1.93223300	2.64355200	H 1.47830900	2.09124500	2.71725500
C 2.71422300	-0.14545100	-3.17782000	H 1.47830900	2.09124500	-2.71725500
C 2.71422300	-0.14545100	3.17782000	C 2.60214800	0.42058900	3.41579800
H 3.61042500	-0.69746900	-3.47665500	C 2.60214800	0.42058900	-3.41579800
H 3.61042500	-0.69746900	3.47665500	H 3.42248800	1.07033600	3.73481000
H 2.86793300	0.22555900	-2.16436600	H 3.42248800	1.07033600	-3.73481000

H 2.86793300	0.22555900	2.16436600	H 2.86493400	-0.00410900	2.44719000
H 2.63127000	0.71565000	-3.84403000	H 2.86493400	-0.00410900	-2.44719000
H 2.63127000	0.71565000	3.84403000	H 2.54008500	-0.39481900	4.13963700
C 1.26006900	-1.53485500	-4.70586100	H 2.54008500	-0.39481900	-4.13963700
C 1.26006900	-1.53485500	4.70586100	C 0.90477600	1.72082400	4.74936900
H 1.10886700	-0.69568100	-5.38934100	C 0.90477600	1.72082400	-4.74936900
H 1.10886700	-0.69568100	5.38934100	H 0.74088900	0.89139800	5.44192800
H 0.39898200	-2.20152600	-4.79136300	H 0.74088900	0.89139800	-5.44192800
H 0.39898200	-2.20152600	4.79136300	H 0.00130700	2.33337600	4.73401400
H 2.13713900	-2.08351100	-5.06233900	H 0.00130700	2.33337600	-4.73401400
H 2.13713900	-2.08351100	5.06233900	H 1.70932300	2.33277200	5.16834100
C -1.15948000	-1.85320100	-2.44380100	H 1.70932300	2.33277200	-5.16834100
C -1.15948000	-1.85320100	2.44380100	C -1.39050800	1.69843600	2.44894600
H -1.75661900	-1.90181400	-3.35713700	C -1.39050800	1.69843600	-2.44894600
H -1.75661900	-1.90181400	3.35713700	H -1.99725300	1.66200500	3.35665600
H -0.50327300	-2.72849000	-2.43216300	H -1.99725300	1.66200500	-3.35665600
H -0.50327300	-2.72849000	2.43216300	H -0.85181300	2.65106000	2.45192100
C -2.04450900	-1.86845700	-1.20233200	H -0.85181300	2.65106000	-2.45192100
C -2.04450900	-1.86845700	1.20233200	H -2.97856900	0.78242000	1.30889000
H -2.85203100	-1.12465200	-1.31792100	H -2.97856900	0.78242000	-1.30889000
H -2.85203100	-1.12465200	1.31792100	H -2.86087400	2.53184200	1.13239000
H -2.54079600	-2.85095500	-1.14225100	H -2.86087400	2.53184200	-1.13239000
H -2.54079600	-2.85095500	1.14225100	O -1.00096400	-2.84173300	0.00000000
2W-cis + PhCN-TS-H_M transfer			2W-trans + PhCN-TS-H_M transfer		
C -2.62525800	-0.53329300	0.00000000	N -2.44486800	-0.73971800	0.00000000
O -3.77857000	-0.70683000	0.00000000	O -3.58743800	-1.08355200	0.00000000
P -0.57654700	0.22302700	2.42705800	W -0.70465300	-0.24388600	0.00000000
P -0.57654700	0.22302700	-2.42705800	P -0.57940100	0.23936500	2.42456600
C -0.73160000	2.08425000	2.45294500	P -0.57940100	0.23936500	-2.42456600
C -0.73160000	2.08425000	-2.45294500	C -0.72165100	2.10434300	2.45901500
H 0.28844000	2.47778100	2.42973700	C -0.72165100	2.10434300	-2.45901500
H 0.28844000	2.47778100	-2.42973700	H 0.29954400	2.49565400	2.44803700
H -1.20352200	2.44726700	3.36771900	H 0.29954400	2.49565400	-2.44803700
H -1.20352200	2.44726700	-3.36771900	H -1.20489300	2.46844500	3.36783700
C -1.47968100	2.58162500	1.22508400	H -1.20489300	2.46844500	-3.36783700
C -1.47968100	2.58162500	-1.22508400	C -1.45436500	2.60009600	1.22162800
H -1.43995600	3.67844500	1.18832000	C -1.45436500	2.60009600	-1.22162800
H -1.43995600	3.67844500	-1.18832000	H -1.40054000	3.69614900	1.17661400
H -2.53149400	2.28859800	1.25624900	H -1.40054000	3.69614900	-1.17661400
H -2.53149400	2.28859800	-1.25624900	H -2.51018400	2.32095500	1.24897500
N -0.87422000	2.02023400	0.00000000	H -2.51018400	2.32095500	-1.24897500
C 1.04940100	-0.02929200	-3.33477300	N -0.85511300	2.02210700	0.00000000
C 1.04940100	-0.02929200	3.33477300	C 1.02258700	-0.01847600	-3.37280100
H 1.74997600	0.46194000	-2.65107700	C 1.02258700	-0.01847600	3.37280100
H 1.74997600	0.46194000	2.65107700	H 1.74222200	0.47546700	-2.71067000
C -1.89040400	-0.43358100	-3.60310300	H 1.74222200	0.47546700	2.71067000
C -1.89040400	-0.43358100	3.60310300	C -1.94788800	-0.38952600	-3.54764200
C -3.21349800	0.31925000	-3.48447800	C -1.94788800	-0.38952600	3.54764200
C -3.21349800	0.31925000	3.48447800	C -3.26927800	0.33939100	-3.31062300
N -0.32246500	-2.03400400	0.00000000	C -3.26927800	0.33939100	3.31062300
O -0.05447200	-3.19143900	0.00000000	C -0.10366000	-2.12153800	0.00000000
C -2.10837100	-1.92888000	3.37273200	O 0.26706700	-3.22432000	0.00000000
C -2.10837100	-1.92888000	-3.37273200	H -1.61356600	-0.17834700	4.56937100
H -1.19310800	-2.51132200	3.47886800	H -1.61356600	-0.17834700	-4.56937100
H -1.19310800	-2.51132200	-3.47886800	C -2.13851900	-1.89727800	3.38447900
H -2.49886800	-2.11087500	2.37003900	C -2.13851900	-1.89727800	-3.38447900
H -2.49886800	-2.11087500	-2.37003900	H -1.22235700	-2.46098000	3.55934800
H -2.83497700	-2.31216000	4.09549900	H -1.22235700	-2.46098000	-3.55934800
H -2.83497700	-2.31216000	-4.09549900	H -2.48937600	-2.13574300	2.37954600
C 1.43987500	-1.50273100	-3.42419500	H -2.48937600	-2.13574300	-2.37954600
C 1.43987500	-1.50273100	3.42419500	H -2.88950200	-2.25037400	4.09777900
H 0.85159000	-2.02597500	-4.18189100	H -2.88950200	-2.25037400	-4.09777900

H 0.85159000	-2.02597500	4.18189100	C 1.41926300	-1.48846900	-3.48046700
H 1.30821300	-2.02047600	-2.47269600	C 1.41926300	-1.48846900	3.48046700
H 1.30821300	-2.02047600	2.47269600	H 0.81746200	-2.01046700	-4.22809400
H 2.49089900	-1.59072800	-3.71318900	H 0.81746200	-2.01046700	4.22809400
H 2.49089900	-1.59072800	3.71318900	H 1.31258000	-2.01252900	-2.53014200
C 1.13975600	0.65332400	-4.69710400	H 1.31258000	-2.01252900	2.53014200
C 1.13975600	0.65332400	4.69710400	H 2.46395800	-1.56666800	-3.79397600
H 0.90842800	1.71928300	-4.65064500	H 2.46395800	-1.56666800	3.79397600
H 0.90842800	1.71928300	4.65064500	C 1.06826700	0.66843300	-4.73559400
H 0.47089200	0.19191500	-5.42819400	C 1.06826700	0.66843300	4.73559400
H 0.47089200	0.19191500	5.42819400	H 0.83712300	1.73368300	-4.67940700
H 2.15669400	0.55767500	-5.08952500	H 0.83712300	1.73368300	4.67940700
H 2.15669400	0.55767500	5.08952500	H 0.37661700	0.20671900	-5.44495700
H 1.12438000	0.36942000	0.00000000	H 0.37661700	0.20671900	5.44495700
H 0.12534800	2.33670900	0.00000000	H 2.07217700	0.57479100	-5.16033100
N 1.89831100	2.57255000	0.00000000	H 2.07217700	0.57479100	5.16033100
C 2.24121600	1.43525000	0.00000000	H 1.17561900	0.32312400	0.00000000
C 3.43349200	0.58191000	0.00000000	H 0.15448900	2.32568900	0.00000000
C 3.36794600	-0.80717800	0.00000000	N 1.89573800	2.50936900	0.00000000
C 4.53448200	-1.56043000	0.00000000	C 2.22535800	1.36249300	0.00000000
C 5.77220300	-0.93060100	0.00000000	C 3.45111100	0.54978500	0.00000000
C 4.68187400	1.21605900	0.00000000	C 3.43286200	-0.84015000	0.00000000
C 5.84226500	0.45971400	0.00000000	C 4.62287700	-1.55623400	0.00000000
H 2.39264100	-1.28090200	0.00000000	C 5.83913900	-0.88622800	0.00000000
H 4.47343800	-2.64286600	0.00000000	C 4.67817400	1.22356000	0.00000000
H 6.68251200	-1.52003200	0.00000000	C 5.86278400	0.50585900	0.00000000
H 4.71970300	2.29891300	0.00000000	H 2.47679500	-1.34981400	0.00000000
H 6.80666700	0.95557500	0.00000000	H 4.59700800	-2.64011900	0.00000000
H -1.49434500	-0.28094400	4.61281800	H 6.76835900	-1.44536300	0.00000000
H -1.49434500	-0.28094400	-4.61281800	H 4.67860800	2.30711100	0.00000000
H -3.93732100	-0.10774100	-4.18500700	H 6.81046900	1.03311100	0.00000000
H -3.93732100	-0.10774100	4.18500700	H -4.02797800	-0.05998300	-3.99019400
H -3.63729200	0.22348200	-2.48336100	H -4.02797800	-0.05998300	3.99019400
H -3.63729200	0.22348200	2.48336100	H -3.63150000	0.18404600	-2.29286300
H -3.11988500	1.38019900	-3.72413500	H -3.63150000	0.18404600	2.29286300
H -3.11988500	1.38019900	3.72413500	H -3.19939400	1.41221600	-3.49987000
W -0.67431200	-0.25624100	0.00000000	H -3.19939400	1.41221600	3.49987000
2W-cis + PhCN-interm			2W-trans + PhCN-interm		
C -2.60524300	-0.56092000	0.00000000	N 0.01142200	-2.43941200	-0.74357000
O -3.75484200	-0.75662900	0.00000000	O 0.01679300	-3.58242900	-1.08473300
W -0.67402100	-0.24961100	0.00000000	W 0.00334200	-0.70643400	-0.24233100
P -0.57571200	0.22509500	2.43358600	P 2.42998400	-0.56529100	0.23968700
P -0.57571200	0.22509500	-2.43358600	P -2.42436700	-0.58806400	0.23994100
C -0.68843600	2.08714600	2.45495100	C 2.46290000	-0.68590100	2.10500100
C -0.68843600	2.08714600	-2.45495100	C -2.45586400	-0.70849600	2.10529500
H 0.34054100	2.45632800	2.43324500	H 2.44726900	0.33977700	2.48399400
H 0.34054100	2.45632800	-2.43324500	H -2.44963000	0.31737700	2.48403000
H -1.15577500	2.46284100	3.36698400	H 3.37312700	-1.16181000	2.47517400
H -1.15577500	2.46284100	-3.36698400	H -3.36160900	-1.19267900	2.47572800
C -1.41852400	2.59664200	1.22118900	C 1.22681100	-1.41628800	2.60739300
C -1.41852400	2.59664200	-1.22118900	C -1.21302800	-1.42732200	2.60772800
H -1.33874600	3.69093600	1.17574300	H 1.17758100	-1.34232900	3.70207000
H -1.33874600	3.69093600	-1.17574300	H -1.16433000	-1.35255800	3.70237400
H -2.48102800	2.34415400	1.25685600	H 1.26190700	-2.47730600	2.34882300
H -2.48102800	2.34415400	-1.25685600	H -1.23840000	-2.48871200	2.34954700
N -0.82988800	2.00808800	0.00000000	N 0.00414500	-0.83215000	-2.01599200
C 1.04442900	-0.06693200	-3.33929900	C -3.37946000	1.00637000	-0.03842000
C 1.04442900	-0.06693200	3.33929900	C 3.37029500	1.03799800	-0.03827300
H 1.75598800	0.41787900	-2.66216200	H -2.72244400	1.73545600	0.44856100
H 1.75598800	0.41787900	2.66216200	H 2.70669300	1.76085800	0.44906000
C -1.90988000	-0.40280100	-3.60054100	C -3.53683600	-1.97090300	-0.37488200
C -1.90988000	-0.40280100	3.60054100	C 3.55506700	-1.93761300	-0.37574200

C -3.21916300	0.37043600	-3.46108200	C -3.28756600	-3.28327400	0.36613100
C -3.21916300	0.37043600	3.46108200	C 3.31854600	-3.25225700	0.36541900
N -0.30906700	-2.02694600	0.00000000	C 0.00053000	-0.10309900	-2.12023900
O -0.03224100	-3.18084600	0.00000000	O -0.00125700	0.26392300	-3.22389700
C -2.14860400	-1.89713600	3.38561400	H 4.57552300	-1.59926700	-0.16475700
C -2.14860400	-1.89713600	-3.38561400	H -4.56029300	-1.64212200	-0.16330400
H -1.24336500	-2.49199400	3.50688600	C 3.39676600	-2.14221700	-1.88212800
H -1.24336500	-2.49199400	-3.50688600	C -3.37749300	-2.17406200	-1.88134600
H -2.53474800	-2.08602000	2.38260300	H 3.56979700	-1.23049300	-2.45345900
H -2.53474800	-2.08602000	-2.38260300	H -3.55935200	-1.26402000	-2.45261700
H -2.88668300	-2.26028700	4.10703400	H 2.39428400	-2.49978200	-2.12077100
H -2.88668300	-2.26028700	-4.10703400	H -2.37186500	-2.52229500	-2.12054300
C 1.41080000	-1.54711400	-3.41968700	H 4.11421300	-2.89336200	-2.22626300
C 1.41080000	-1.54711400	3.41968700	H -4.08809700	-2.93188600	-2.22504100
H 0.81352400	-2.06590000	-4.17327200	C -3.48853100	1.38680100	-1.51261500
H 0.81352400	-2.06590000	4.17327200	C 3.47562500	1.41993600	-1.51234500
H 1.27399900	-2.05765400	-2.46508300	H -4.23273500	0.77569100	-2.02859700
H 1.27399900	-2.05765400	2.46508300	H 4.22513900	0.81572100	-2.02875800
H 2.45984800	-1.65247200	-3.70962300	H -2.53763100	1.28063900	-2.03573400
H 2.45984800	-1.65247200	3.70962300	H 2.52557200	1.30543100	-2.60322200
C 1.14301200	0.60568000	-4.70620500	H -3.80763700	2.42890000	-1.60130800
C 1.14301200	0.60568000	4.70620500	H 3.78533200	2.46489100	-1.60073700
H 0.92849700	1.67536800	-4.66598500	C -4.74291500	1.05177800	0.64737300
H 0.92849700	1.67536800	4.66598500	C 4.73334500	1.09565900	0.64738000
H 0.46620100	0.14956500	-5.43327400	H -4.68591900	0.83301300	1.71516300
H 0.46620100	0.14956500	5.43327400	H 4.67848400	0.87565900	1.71502600
H 2.15792300	0.49177300	-5.09865100	H -5.44810800	0.35114700	0.19286500
H 2.15792300	0.49177300	5.09865100	H 5.44497500	0.40191600	0.19233900
H 1.19151600	0.42144800	0.00000000	H -5.17288100	2.05226400	0.54233000
H 0.20058800	2.32140100	0.00000000	H 5.15396700	2.10017300	0.54294800
N 1.85220000	2.51002200	0.00000000	H -0.00560100	1.20986500	0.35575400
C 2.14225300	1.33744700	0.00000000	H -0.00047900	0.19314500	2.31542400
C 3.39602100	0.55409600	0.00000000	N -0.00835600	1.87568300	2.47969500
C 3.38889200	-0.83652200	0.00000000	C -0.01005300	2.17795400	1.31463100
C 4.58406200	-1.54454000	0.00000000	C -0.01626800	3.43307700	0.53576400
C 5.79467500	-0.86386000	0.00000000	C -0.01683900	3.44269200	-0.85431500
C 4.61610900	1.23707600	0.00000000	C -0.02283300	4.64587600	-1.54862300
C 5.80670500	0.52879300	0.00000000	C -0.02830300	5.84868800	-0.85470600
H 2.43565000	-1.35576800	0.00000000	C -0.02180400	4.64613600	1.23237900
H 4.56815100	-2.62876800	0.00000000	C -0.02777100	5.84461700	0.53789800
H 6.72863400	-1.41517200	0.00000000	H -0.01256200	2.49763400	-1.38555800
H 4.60396800	2.32085700	0.00000000	H -0.02322500	4.64153000	-2.63291000
H 6.75078400	1.06276900	0.00000000	H -0.03298800	6.78876500	-1.39543400
H -1.52047700	-0.24439700	4.61192900	H -0.02131400	4.62246600	2.31585600
H -1.52047700	-0.24439700	-4.61192900	H -0.03204600	6.78222600	1.08307200
H -3.95565200	-0.03574700	-4.16067800	H -3.96218900	-4.05099300	-0.02421800
H -3.95565200	-0.03574700	4.16067800	H 4.00013000	-4.01361300	-0.02530100
H -3.63635400	0.26955400	-2.45772400	H -2.26740200	-3.63914100	0.21188300
H -3.63635400	0.26955400	2.45772400	H 2.30167600	-3.61768400	0.21177200
H -3.10913900	1.43245200	-3.68823400	H -3.47458100	-3.20425500	1.43865900
H -3.10913900	1.43245200	3.68823400	H 3.50541700	-3.17145500	1.43783900
2W-cis + PhCN-TS-H_M transfer			2W-trans + PhCN-TS-H_M transfer		
C -2.61583300	-0.58136000	0.00000000	N -0.76973700	-2.44946200	0.00000000
O -3.76237700	-0.79314200	0.00000000	O -1.11097600	-3.59253800	0.00000000
W -0.70212200	-0.23979000	0.00000000	W -0.23311000	-0.73774200	0.00000000
P -0.59431500	0.22297300	2.43933900	P 0.23609800	-0.59502400	-2.43333000
P -0.59431500	0.22297300	-2.43933900	P 0.23609800	-0.59502400	2.43333000
C -0.57505600	2.08525600	2.46011300	C 2.10067400	-0.55446900	-2.46560400
C -0.57505600	2.08525600	-2.46011300	C 2.10067400	-0.55446900	2.46560400
H 0.47752600	2.37992300	2.46122900	H 2.38888600	0.49985300	-2.48495200
H 0.47752600	2.37992300	-2.46122900	H 2.38888600	0.49985300	2.48495200
H -1.03354900	2.49314700	3.36300400	H 2.50937900	-1.02554500	-3.36198500

H -1.03354900	2.49314700	-3.36300400	H 2.50937900	-1.02554500	3.36198500
C -1.24179700	2.63941000	1.20908000	C 2.65927900	-1.19918700	-1.20583600
C -1.24179700	2.63941000	-1.20908000	C 2.65927900	-1.19918700	1.20583600
H -1.04308200	3.71882100	1.14808200	H 3.73418500	-0.97824600	-1.13948400
H -1.04308200	3.71882100	-1.14808200	H 3.73418500	-0.97824600	1.13948400
H -2.32848500	2.51463300	1.25687800	H 2.55709000	-2.28858300	-1.24626400
H -2.32848500	2.51463300	-1.25687800	H 2.55709000	-2.28858300	1.24626400
N -0.71796600	1.97629200	0.00000000	N 1.97881100	-0.68789600	0.00000000
C 0.99970400	-0.18404200	-3.34878800	C -0.17954000	0.96442300	3.39854700
C 0.99970400	-0.18404200	3.34878800	C -0.17954000	0.96442300	-3.39854700
H 1.74065200	0.28529500	-2.69207500	H 0.27323500	1.73275300	2.76154800
H 1.74065200	0.28529500	2.69207500	H 0.27323500	1.73275300	-2.76154800
C -1.97928900	-0.30076500	-3.59570500	C -0.25735300	-2.03741200	3.52724300
C -1.97928900	-0.30076500	3.59570500	C -0.25735300	-2.03741200	-3.52724300
C -3.24362600	0.53198000	-3.39521400	C 0.55815200	-3.29096500	3.21496400
C -3.24362600	0.53198000	3.39521400	C 0.55815200	-3.29096500	-3.21496400
N -0.32914100	-2.01988800	0.00000000	C -2.10337900	-0.10331000	0.00000000
O -0.03286100	-3.16904100	0.00000000	O -3.19958900	0.28577500	0.00000000
C -2.28786300	-1.78860900	3.43339900	H -0.02788400	-1.72051500	-4.55059100
C -2.28786300	-1.78860900	-3.43339900	H -0.02788400	-1.72051500	4.55059100
H -1.41864700	-2.42220100	3.60927600	C -1.75279700	-2.33317800	-3.41819700
H -1.41864700	-2.42220100	-3.60927600	C -1.75279700	-2.33317800	3.41819700
H -2.65362900	-2.00077400	2.42750600	H -2.37318700	-1.46767300	-3.64962600
H -2.65362900	-2.00077400	-2.42750600	H -2.37318700	-1.46767300	3.64962600
H -3.06518300	-2.08350600	4.14460600	H -2.01034100	-2.67106100	-2.41377100
H -3.06518300	-2.08350600	-4.14460600	H -2.01034100	-2.67106100	2.41377100
C 1.29724100	-1.68122200	-3.38907700	H -2.01841200	-3.13032600	-4.11913700
C 1.29724100	-1.68122200	3.38907700	H -2.01841200	-3.13032600	4.11913700
H 0.67582600	-2.19285300	-4.12756800	C -1.67677500	1.25027600	3.47946900
H 0.67582600	-2.19285300	4.12756800	C -1.67677500	1.25027600	-3.47946900
H 1.13909900	-2.15986700	-2.42158100	H -2.16764100	0.60612600	4.21239900
H 1.13909900	-2.15986700	2.42158100	H -2.16764100	0.60612600	-4.21239900
H 2.33962700	-1.84205300	-3.67799600	H -2.17543800	1.11499400	2.51938800
H 2.33962700	-1.84205300	3.67799600	H -2.17543800	1.11499400	-2.51938800
C 1.11942800	0.44592800	-4.73427400	H -1.83663200	2.28349200	3.80009700
C 1.11942800	0.44592800	4.73427400	H -1.83663200	2.28349200	-3.80009700
H 0.94704000	1.52400300	-4.72319400	C 0.47384200	1.03944300	4.77683600
H 0.94704000	1.52400300	4.72319400	C 0.47384200	1.03944300	-4.77683600
H 0.42161800	-0.00358500	-5.44526600	H 1.55389900	0.88569300	4.74112000
H 0.42161800	-0.00358500	5.44526600	H 1.55389900	0.88569300	-4.74112000
H 2.12717300	0.28074100	-5.12692600	H 0.04740700	0.30595300	5.46584600
H 2.12717300	0.28074100	5.12692600	H 0.04740700	0.30595300	-5.46584600
H 1.28784300	0.33715500	0.00000000	H 0.29923600	2.02768400	5.21242400
H 0.46647100	2.27093200	0.00000000	H 0.29923600	2.02768400	-5.21242400
N 1.83318300	2.38829200	0.00000000	H 0.29640900	1.32372300	0.00000000
C 2.14517000	1.20149500	0.00000000	H 2.25089300	0.50709800	0.00000000
C 3.45415600	0.51511400	0.00000000	N 2.35169200	1.86683300	0.00000000
C 3.52978100	-0.87518600	0.00000000	C 1.16511000	2.18025100	0.00000000
C 4.76469400	-1.51138900	0.00000000	C 0.49115300	3.49623400	0.00000000
C 5.93204900	-0.75880400	0.00000000	C -0.89765000	3.59262700	0.00000000
C 4.63106700	1.26874200	0.00000000	C -1.51619600	4.83661600	0.00000000
C 5.86148100	0.63238800	0.00000000	C -0.74735000	5.99311600	0.00000000
H 2.61178900	-1.45527600	0.00000000	C 1.26101200	4.66291100	0.00000000
H 4.81437000	-2.59458300	0.00000000	C 0.64264600	5.90231300	0.00000000
H 6.89724800	-1.25336100	0.00000000	H -1.49350000	2.68577500	0.00000000
H 4.55304800	2.34990700	0.00000000	H -2.59858500	4.90124200	0.00000000
H 6.77275800	1.22059500	0.00000000	H -1.22809700	6.96525100	0.00000000
H -1.60426200	-0.12090300	4.60892800	H 2.34090100	4.56931300	0.00000000
H -1.60426200	-0.12090300	-4.60892800	H 1.24412800	6.80488000	0.00000000
H -4.01609900	0.19003000	-4.09033500	H 0.23831800	-4.10265600	3.87502900
H -4.01609900	0.19003000	4.09033500	H 0.23831800	-4.10265600	-3.87502900
H -3.64142800	0.41618800	-2.38571600	H 0.39774200	-3.62400200	2.18808500
H -3.64142800	0.41618800	2.38571600	H 0.39774200	-3.62400200	-2.18808500

H -3.08320300	1.59457900	-3.58617600	H 1.62833800	-3.14673500	3.37363600
H -3.08320300	1.59457900	3.58617600	H 1.62833800	-3.14673500	-3.37363600
2W-cis + PhCHNH-TS			2W-trans + PhCHNH-TS		
N 0.52838700	-0.49048200	2.01583400	N 0.53299300	-0.45951100	2.01418400
H -0.67546600	1.04298000	0.28662600	H -0.72517000	1.05911400	0.24718000
H -0.09491200	0.34339200	2.30006800	H -0.08577500	0.40079700	2.27907400
C -1.10646700	2.07147800	1.21235800	C -1.10938700	2.06513800	1.13057100
N -1.12380600	1.64632800	2.47684300	N -1.06761200	1.68710200	2.41895500
C -2.33490500	2.54862300	0.48292300	C -2.38173600	2.51714300	0.45545600
C -2.32762500	2.71410000	-0.90287600	C -2.42514200	2.71321100	-0.92559500
C -3.43317800	3.22893600	-1.56211100	C -3.57110600	3.19356300	-1.54053000
C -4.57191800	3.58460200	-0.84525100	C -4.70037800	3.48692700	-0.78198000
C -4.58922400	3.42675600	0.53344800	C -4.66656700	3.30239100	0.59301100
C -3.47518300	2.91865800	1.19357700	C -3.51258900	2.82724000	1.20773100
P 2.45049900	1.02132100	0.20088400	P 2.45617300	1.03749300	0.21990400
P -1.53338800	-1.78942200	0.20513100	P -1.50811100	-1.79481600	0.22331400
N 0.31828600	-0.18697500	-2.04375700	C -3.22190500	-1.11914200	-0.13873600
C 1.60730000	-2.02446100	-0.48321400	C 2.44658000	2.87552900	-0.18776800
C -3.22481000	-1.04814400	-0.12866800	C -1.54531900	-3.59455000	-0.31451600
C 2.39371100	2.85241000	-0.23032300	C 4.16540700	0.43669400	-0.27856200
C -1.66827400	-3.56750900	-0.39732600	O 2.16777600	-2.79618800	-1.08226500
C 4.18495600	0.48915200	-0.30315500	C 2.46912600	1.07519400	2.08781200
O 2.26080800	-2.97897900	-0.63538900	C -1.51784500	-1.83892400	2.09223500
C 2.44450900	1.06089100	2.06656800	H 1.85860400	1.93055500	2.39211900
C -1.51335000	-1.86943400	2.07034600	H -2.15445700	-1.01131300	2.41688000
H 1.81204000	1.90395200	2.35983100	H 3.47220000	1.22202400	2.49419100
H -2.13741500	-1.04096000	2.41555200	H -1.95523500	-2.75902100	2.48520600
H 3.43940600	1.23563600	2.48112200	C 1.84440800	-0.19653300	2.64294400
H -1.95749500	-2.79084300	2.45103300	C -0.11244700	-1.63343700	2.63686500
C 1.84485500	-0.22050900	2.62865500	H 1.71528000	-0.09187000	3.72873400
C -0.10176500	-1.68701100	2.60853000	H -0.15978200	-1.49286000	3.72574300
H 1.72943000	-0.12096000	3.71622100	H 2.49151500	-1.05994100	2.46920300
H -0.13754000	-1.58259400	3.70166000	H 0.50971200	-2.51210900	2.44773800
H 2.50003900	-1.07495700	2.44239100	H -3.15323400	-0.11325900	0.29037800
H 0.51743800	-2.55871600	2.38220500	H 1.51526700	3.19918700	0.28893200
H -3.11570800	-0.05111600	0.31159500	C -0.57530800	-4.45869500	0.48929000
H 1.43266800	3.14999200	0.20089300	C 4.62419000	-0.76411800	0.54649000
C -0.82485300	-4.53974800	0.42446900	O -0.07214200	0.36124900	-3.21674000
C 4.74406000	-0.62169000	0.58268800	H 4.83939900	1.27372600	-0.06710000
O 0.18646600	0.00522300	-3.20701400	H -2.56540300	-3.93848700	-0.11037100
H 4.81361200	1.37666200	-0.17584700	C 4.22617100	0.11463500	-1.77156900
H -2.72243400	-3.83958400	-0.27716300	C -1.26353100	-3.73101000	-1.81094400
C 4.21517400	0.06676900	-1.77173400	H 3.92394900	0.95411300	-2.39732500
C -1.29822100	-3.66179100	-1.87767800	H -1.93781800	-3.13407100	-2.42433500
H 3.84861100	0.84327700	-2.44300700	H 3.58365000	-0.73194200	-2.01475200
H -1.88801800	-2.99311300	-2.50451600	H -0.24232000	-3.42776500	-2.04372000
H 3.60402000	-0.82230000	-1.93212900	H 5.25169700	-0.15191500	-2.04492300
H -0.24696000	-3.41390100	-2.03088500	H -1.37944700	-4.77751900	-2.10922000
H 5.24203900	-0.17131100	-2.06522400	C -3.49617200	-0.96158200	-1.63204900
H -1.45988800	-4.68396100	-2.23317700	C 2.32053500	3.15947500	-1.68238000
C -3.48699700	-0.86324800	-1.62138100	H -3.70695000	-1.92435100	-2.10358500
C 2.31412600	3.09569600	-1.73595500	H 3.26599900	2.99230600	-2.20280600
H -3.71254200	-1.81499000	-2.10881300	H -2.66001700	-0.49723700	-2.15560000
H 3.28141800	2.93766600	-2.21814200	H 1.55859600	2.53856300	-2.15510400
H -2.63672800	-0.40780600	-2.13141300	H -4.37544400	-0.32861400	-1.77743400
H 1.58247800	2.44593800	-2.21927900	H 2.04924800	4.20765900	-1.83766000
H -4.35198600	-0.21051100	-1.76499700	C -4.35722800	-1.86783700	0.55551500
H 2.02491700	4.13287200	-1.92856100	C 3.59002400	3.66999800	0.43891500
C -4.38790000	-1.76093300	0.55634500	H -4.21223300	-1.95239900	1.63422500
C 3.48230200	3.70293000	0.41922700	H 3.67327600	3.50952900	1.51551300
H -4.24235200	-1.86985600	1.63307400	H -4.48532900	-2.87501900	0.15051200
H 3.52792000	3.57164300	1.50216000	H 4.55167300	3.42438900	-0.01819200

H -4.56042500	-2.75515600	0.13608200	H -5.29897900	-1.33524300	0.39387500
H 4.47042900	3.48293200	0.00775400	H 3.42467500	4.73979800	0.28003800
H -5.30742800	-1.18698300	0.40807200	H -1.55416200	2.46618700	-1.52361200
H 3.28540300	4.76196200	0.22676500	H -3.58590100	3.33531600	-2.61568000
H -1.45135200	2.40818200	-1.46535700	H -5.59791600	3.86174400	-1.26152500
H -3.41060000	3.34635000	-2.64007800	H -3.47976700	2.72563100	2.28676000
H -5.43813100	3.98505200	-1.36042000	H -5.53620300	3.54203000	1.19549400
H -3.47849400	2.83622100	2.27488700	H 5.62272100	-1.06569300	0.21638600
H -5.46719300	3.71257800	1.10277800	H -0.64065200	-5.49348000	0.14011800
H 5.75017500	-0.88344100	0.24176900	H 4.69088300	-0.53952800	1.61266900
H -0.94820500	-5.55110100	0.02569200	H -0.80057700	-4.46399700	1.55743100
H 4.82500500	-0.32521300	1.63017300	H 3.96379700	-1.62133300	0.40689600
H -1.11747200	-4.57032800	1.47570700	H 0.45688300	-4.13374700	0.34859200
H 4.13686900	-1.52602800	0.52076800	H -0.28314900	2.72163700	0.84621200
H 0.23721300	-4.29693800	0.36480200	H -1.97680300	1.32389500	2.70349700
H -0.24764800	2.70180800	0.97483700	W 0.51271300	-0.44192900	-0.24313100
H -2.04842000	1.28312400	2.70867300	C 0.15282200	0.05065400	-2.11922600
W 0.48757900	-0.42985400	-0.25397800	N 1.52195400	-1.85404000	-0.73500500
2W-cis + PhCHNCH₂Ph-TS			2W-trans + PhCHNCH₂Ph -TS		
O -2.72883500	0.27038300	2.75967900	C 2.02091800	-0.13556800	1.93925500
W -1.18324000	0.48196800	0.19789500	O 2.48410400	0.07032300	2.98466400
P 0.51537300	2.16514100	0.85598000	W 1.20876800	-0.46836300	0.17199200
P -2.34016000	-1.25269000	-1.15548800	P -0.42657300	-2.23122700	0.77822100
C 1.61590700	2.19207000	-0.65252500	P 2.28380200	1.35093800	-1.14246700
C -1.19016000	-1.37524300	-2.62316400	C -1.54284000	-2.25635800	-0.72165300
H 2.43853100	1.50149900	-0.45926200	C 1.13468100	1.46676100	-2.61484900
H -0.44173500	-2.13422300	-2.37795200	H -2.39491800	-1.60934700	-0.50465000
H 2.06055100	3.17412700	-0.82067600	H 0.36672300	2.20552000	-2.36668900
H -1.70586500	-1.70893400	-3.52592900	H -1.94317100	-3.25184800	-0.92276400
C 0.86074700	1.73219700	-1.89093800	H 1.64622300	1.81866100	-3.51365000
C -0.48708200	-0.04730300	-2.87203000	C -0.80704400	-1.72260900	-1.94120300
H 1.56662100	1.61489100	-2.72310700	C 0.46891600	0.12263300	-2.87628800
H 0.26556600	-0.17415300	-3.66102500	H -1.51764600	-1.59769800	-2.76842800
H 0.11382300	2.47222100	-2.18880500	H -0.29895700	0.24029500	-3.65214200
H -1.19682100	0.70977300	-3.21296600	H -0.03586000	-2.42485200	-2.26727700
N 0.16582000	0.45013700	-1.64182800	H 1.19681600	-0.60493700	-3.24176800
C -2.44930400	-3.03642600	-0.55987600	N -0.14958700	-0.42842900	-1.64985100
C 1.72765000	1.78699600	2.24209100	C 2.35648300	3.14239700	-0.56101700
H -1.43343100	-3.22910400	-0.20412800	C -1.65862600	-1.99579700	2.17895000
H 2.01476000	0.75679400	2.00914100	H 1.32021700	3.33136900	-0.26532200
C -4.05727000	-0.93287300	-1.86404500	H -2.01766600	-0.97967900	1.98504500
C 0.01932500	3.95380600	1.18385100	C 3.98876500	1.03207700	-1.87034700
C -4.04667400	0.00401800	-3.06969600	C 0.18067900	-4.00143400	0.96793700
C -0.21475200	4.76108800	-0.09114600	C 3.97037800	-0.00756300	-2.98910800
O -3.03734200	2.73438900	-0.93125700	C 0.56709500	-4.63759700	-0.36636400
C -1.21259400	4.01738000	2.08713800	N 2.48276800	-1.67211000	-0.25967900
C -5.00217100	-0.40092400	-0.78622500	O 3.32917500	-2.47555300	-0.51344300
H -1.08848100	3.45763200	3.01396200	C 1.34570000	-4.09053700	1.95429000
H -5.04422700	-1.04073300	0.09474800	C 4.99216800	0.63197000	-0.78810500
H -2.08938900	3.61721400	1.57711100	H 1.11587300	-3.64913100	2.92339600
H -4.69700100	0.59244600	-0.45692900	H 5.04331200	1.35066900	0.02899200
H -1.42132600	5.05886500	2.35021200	H 2.22956500	-3.58951800	1.55955000
H -6.01514700	-0.32436500	-1.19301100	H 4.74282500	-0.34032300	-0.36378900
C -3.37873200	-3.18350000	0.64361700	H 1.60166300	-5.14174400	2.11914700
C 1.04624400	1.77649900	3.60876700	H 5.99077000	0.55896300	-1.22985000
H -4.42904800	-3.12290300	0.34961400	C 3.21823600	3.32740400	0.68608200
H 0.82711500	2.78988900	3.95362700	C -0.99493500	-1.99514000	3.55404700
H -3.18802600	-2.42364700	1.40357200	H 4.28312000	3.30097200	0.44541100
H 0.11261200	1.21091700	3.59897300	H -0.73545300	-3.00759800	3.87161800
H -3.22922400	-4.16365000	1.10516900	H 3.01606700	2.56554000	1.44004200
H 1.70934400	1.31904500	4.34830200	H -0.08770600	-1.38927800	3.57411100
C -2.77144500	-4.05890300	-1.64671500	H 3.01303700	4.30471200	1.13193800

C 2.98292400	2.65517000	2.25503800	H -1.68821000	-1.59132300	4.29715200
H -2.08005200	-4.00782200	-2.49010400	C 2.72170200	4.14920100	-1.64931000
H 3.51956300	2.63454400	1.30463000	C -2.85177300	-2.94758300	2.14300700
H -3.78693400	-3.93951300	-2.03255800	H 2.08409000	4.06593000	-2.53153300
H 2.75456200	3.69757600	2.49179500	H -3.38151200	-2.92498800	1.18908400
H -2.70498900	-5.06892600	-1.23107500	H 3.76119700	4.04330800	-1.96910200
H 3.67049500	2.29603300	3.02687600	H -2.55249000	-3.98008500	2.34043100
H 0.19978000	-0.84597500	0.60956800	H 2.60973300	5.16568100	-1.26032000
H 0.91356000	-0.26207400	-1.40353400	H -3.56787200	-2.66827200	2.92172200
N 1.98071700	-1.54720900	-0.72939400	H -0.23325000	0.81688500	0.69333700
H 0.86877700	4.39530600	1.71611400	H -0.92027100	0.25433700	-1.38474600
H -4.41873200	-1.91161000	-2.19670900	N -2.00281800	1.47251100	-0.67180100
H -5.07037600	0.13500600	-3.43288300	H -0.67288400	-4.55400300	1.37628300
H -0.49393000	5.78442400	0.17713400	H 4.29724000	1.99018500	-2.30215500
H -3.67088700	0.99333800	-2.80436000	H 4.98637300	-0.13686800	-3.37385800
H -1.03367400	4.34887900	-0.68225700	H 0.89303100	-5.66722500	-0.19118800
H -3.45660900	-0.38384900	-3.90217000	H 3.63629800	-0.98053200	-2.62574600
H 0.67369800	4.82525000	-0.72182100	H 1.40010800	-4.11030100	-0.83342800
C 3.25261900	-1.07835400	-0.23207900	H 3.34295900	0.29122200	-3.83103100
H 3.14362600	-0.27116500	0.51252200	H -0.26466100	-4.67912700	-1.07187000
H 3.78656200	-1.87190500	0.31266100	C -3.26747500	0.96648700	-0.19428400
C 4.16525600	-0.58822000	-1.33306600	H -3.14752300	0.12439500	0.51008700
C 3.95695800	-0.94280000	-2.66373400	H -3.80833100	1.72722100	0.38995100
C 5.26982100	0.20654600	-1.02199600	C -4.17680700	0.51753900	-1.31507400
C 4.82942200	-0.51284000	-3.65785600	C -3.98292500	0.94721300	-2.62566800
H 3.10101500	-1.56362800	-2.89952100	C -5.26365000	-0.31476000	-1.04242100
C 6.14215000	0.63808200	-2.01203900	C -4.85267300	0.55484100	-3.63743400
H 5.45037000	0.48812800	0.01188000	H -3.13978300	1.59551700	-2.83181600
C 5.92422300	0.27952100	-3.33778200	C -6.13345400	-0.70884600	-2.05019400
H 4.65422300	-0.80214300	-4.68900600	H -5.43226600	-0.65600300	-0.02460900
H 6.99430600	1.25580500	-1.74905600	C -5.93034700	-0.27470500	-3.35549600
H 6.60380100	0.61511700	-4.11344200	H -4.68880400	0.90248000	-4.65230500
C 1.08220700	-1.94944500	0.16326800	H -6.97185500	-1.35665700	-1.81707100
H 0.25778100	-2.48934500	-0.29991000	H -6.60788000	-0.58099800	-4.14495900
C 1.42881700	-2.55223000	1.50486100	C -1.12392200	1.87899100	0.24339000
C 2.27636400	-3.66512900	1.51414400	H -0.31233400	2.45685800	-0.19752100
C 0.88717800	-2.11947200	2.71102700	C -1.52559400	2.46035500	1.58007400
C 2.58275100	-4.31436600	2.70144800	C -2.32209600	3.61039200	1.56432100
H 2.68864800	-4.02451200	0.57709800	C -1.10820700	1.95837300	2.80770000
C 1.18994800	-2.77190600	3.90129400	C -2.69495900	4.23190500	2.74712600
H 0.21645500	-1.26787100	2.70684700	H -2.64699400	4.01540000	0.61151700
C 2.04172000	-3.86774300	3.90204300	C -1.47792300	2.58242500	3.99464100
H 3.24223800	-5.17552300	2.68852500	H -0.48059500	1.07552400	2.82846500
H 0.75460900	-2.42020700	4.83039700	C -2.27390800	3.71872000	3.96925100
H 2.28038800	-4.37467100	4.83054300	H -3.31277900	5.12292600	2.71482300
N -2.13088600	0.36694900	1.74012200	H -1.13729800	2.17739400	4.94136300
C -2.34472500	1.89063900	-0.51869300	H -2.56374100	4.20448100	4.89446300
2W-cis + PhCHNPh-TS			2W-trans + PhCHNPh-TS		
O 1.84389900	0.13717700	-3.17139300	O 1.49093000	0.16904100	3.32593700
W 1.08590000	0.40843400	-0.28322700	W 1.09827500	-0.40615500	0.27077700
P -0.48613800	2.32008800	-0.40548400	P -0.44414600	-2.34141500	0.39140000
P 2.33384700	-1.52350000	0.66352200	P 2.30733200	1.54783100	-0.68902400
C -1.16369100	2.34606600	1.33355600	C -1.11178600	-2.40389100	-1.35364800
C 1.67359200	-1.55127200	2.41244600	C 1.66709800	1.55122500	-2.44892100
H -2.06008000	1.72014700	1.32650900	H -2.03167900	-1.81270900	-1.36273400
H 0.79421800	-2.20234300	2.40912500	H 0.78622300	2.20030800	-2.47112200
H -1.47165000	3.34674800	1.64221200	H -1.37600300	-3.41810800	-1.66044500
H 2.38898600	-1.97739100	3.11839000	H 2.39180200	1.96355800	-3.15432400
C -0.15400200	1.77478200	2.31976200	C -0.10922500	-1.80188800	-2.32776900
C 1.25368500	-0.15576200	2.85568000	C 1.26022000	0.14460500	-2.86732400
H -0.61585900	1.69300800	3.31231200	H -0.56425400	-1.72713400	-3.32426000
H 0.77240900	-0.21342500	3.84085100	H 0.77709500	0.18100100	-3.85283200

H 0.71495300	2.43065300	2.41259700	H 0.77630800	-2.43567000	-2.41540300
H 2.12088900	0.50142700	2.94879100	H 2.13478500	-0.50379200	-2.95165700
N 0.32094900	0.44500200	1.87920400	N 0.33848000	-0.46280700	-1.88265600
C 2.02229500	-3.28874400	0.08083200	C 1.99953300	3.33155900	-0.16148500
C -2.04080300	2.16834200	-1.44455700	C -2.02259200	-2.26874300	1.40387100
H 0.93032200	-3.34314700	0.05396200	H 0.90816500	3.40190400	-0.19655900
H -2.40072800	1.18372900	-1.13452900	H -2.44141800	-1.31842600	1.06151200
C 4.21280500	-1.45932200	0.81274700	C 4.17947400	1.43639500	-0.84502400
C 0.12747300	4.06605500	-0.75695000	C 0.26302000	-4.05440600	0.70816700
C 4.69885300	-0.59218500	1.97172000	C 4.62953900	0.43623600	-1.90805600
C 0.80042100	4.72498800	0.44505200	C 1.07615500	-4.58617200	-0.47064400
O 3.46567700	2.35257700	0.32754400	O 3.52435400	-2.17419600	0.20617300
C 1.06345400	4.07822200	-1.96574000	C 1.09862300	-4.08108300	1.98819200
C 4.84693000	-0.99782900	-0.49965600	C 4.83166300	1.11345400	0.49972300
H 0.61694100	3.62544700	-2.85090100	H 0.55074400	-3.71909600	2.85780200
H 4.53270200	-1.59454700	-1.35568000	H 4.53954600	1.80522800	1.28905200
H 1.98547100	3.53750300	-1.74948300	H 1.99617100	-3.47181000	1.88060000
H 4.59105800	0.04044400	-0.71173500	H 4.57536300	0.10593300	0.82648000
H 1.32846200	5.11021800	-2.21526300	H 1.41306700	-5.10840400	2.19664200
H 5.93636900	-1.06803700	-0.42434800	H 5.91986200	1.16639000	0.39621300
C 2.51737800	-3.51163800	-1.34700000	C 2.42076500	3.59852300	1.28191700
C -1.73273200	2.10310500	-2.93881300	C -1.76533300	-2.15159700	2.90396700
H 3.60639000	-3.58868000	-1.38580500	H 3.50536200	3.69015100	1.37202400
H -1.46741200	3.08552400	-3.33670700	H -1.46754900	-3.10953000	3.33632300
H 2.20487900	-2.70950200	-2.01814400	H 2.08490900	2.81115800	1.95817000
H -0.91710600	1.41278300	-3.16084100	H -0.99051700	-1.41858600	3.13155900
H 2.11311100	-4.45081900	-1.73493900	H 1.98773900	4.54311500	1.62269000
H -2.61862600	1.76371600	-3.48313600	H -2.68351100	-1.84146000	3.41102200
C 2.52249400	-4.37887400	1.02531300	C 2.56235500	4.38468900	-1.11316200
C -3.12328700	3.19972700	-1.14059500	C -3.02747400	-3.37491300	1.09431300
H 2.13234000	-4.26827600	2.03895900	H 2.23252000	4.24067800	-2.14378400
H -3.40305600	3.21558300	-0.08587300	H -3.27234300	-3.43515400	0.03258900
H 3.61356400	-4.40221700	1.08220200	H 3.65488100	4.39921500	-1.10412100
H -2.81933300	4.20874200	-1.43125800	H -2.66803300	-4.35407200	1.42115000
H 2.20141700	-5.35812200	0.65745000	H 2.22757100	5.37789200	-0.79926200
H -4.02599100	2.96258400	-1.71173900	H -3.96093700	-3.18226900	1.63144800
H -0.54042900	-0.63420700	-0.35325300	H -0.56766100	0.63663200	0.40336500
H -0.51488400	-0.18171000	1.85756100	H -0.50992100	0.14942200	-1.86601300
N -1.94169300	-1.33537900	1.51441900	N -1.94114400	1.27132300	-1.50566200
H -0.77098500	4.64234500	-1.00196600	H -0.60959600	-4.70324700	0.84076200
H 4.52196300	-2.49144800	1.00792600	H 4.49857000	2.43505000	-1.16177000
H 5.79228100	-0.61432300	2.00361400	H 5.72260800	0.43279900	-1.95529500
H 1.11419600	5.73713500	0.17242200	H 1.44285100	-5.58868200	-0.23039800
H 4.40242800	0.44992900	1.84449000	H 4.31406200	-0.57866200	-0.66209800
H 1.69593800	4.18238200	0.75112400	H 1.94868400	-3.96192600	-1.66854200
H 4.34152200	-0.94284000	2.94179900	H 4.26552100	0.68912200	-2.90571800
H 0.13451200	4.81546700	1.30524300	H 0.48600500	-4.67040100	-1.38519300
C -1.44379100	-1.77916200	0.37527200	C -1.45226100	1.74116100	-0.37125000
H -0.52744800	-2.34147600	0.52533500	H -0.53906700	2.30839900	-0.52819500
C -2.20351500	-2.31027400	-0.80856900	C -2.23723700	2.31232300	0.77886500
C -3.26793800	-3.18461600	-0.56934200	C -3.28248500	3.19195900	0.48100700
C -1.80287100	-2.08639300	-2.12409200	C -1.88782000	2.11563500	2.11254100
C -3.92219800	-3.80571000	-1.62341300	C -3.96631800	3.84598100	1.49549100
H -3.58069600	-3.37377800	0.45112100	H -3.55731400	3.35786600	-0.55429400
C -2.45857600	-2.70978300	-3.17888700	C -2.57334800	2.77135700	3.12820000
H -0.97705400	-1.40964100	-2.31142700	H -1.07988300	1.43440700	2.35002200
C -3.52187600	-3.56871100	-2.93344400	C -3.61601000	3.63661800	2.82440400
H -4.74757500	-4.47922800	-1.41962400	H -4.77604300	4.52306900	1.24591900
H -2.13579300	-2.51935800	-4.19667100	H -2.28954800	2.60110000	4.16101900
H -4.03559600	-4.05202600	-3.75717200	H -4.15279900	4.14556900	3.61737800
C -3.18940600	-0.73272500	1.65157600	C -3.18279600	0.65568900	-1.63055400
C -3.63963400	-0.55566800	2.97288600	C -3.63065200	0.44118400	-2.94730500
C -4.02027100	-0.25841900	0.62100900	C -4.00985200	0.19922900	-0.58857900

C -4.85374000	0.04738800	3.25213300	C -4.83825000	-0.18126400	-3.21152800
H -3.00439200	-0.91998800	3.77289700	H -2.99911000	0.79181900	-3.75636300
C -5.23589600	0.34952700	0.90768400	C -5.21857600	-0.42895800	-0.86042500
H -3.72308100	-0.38124200	-0.41120600	H -3.71496100	0.35177700	0.44053000
C -5.66534400	0.50772000	2.21912100	C -5.64552800	-0.62450300	-2.16760400
H -5.17132700	0.15973600	4.28358100	H -5.15414500	-0.32259400	-4.23993600
H -5.85699900	0.70026300	0.08988000	H -5.83655700	-0.76553300	-0.03430800
H -6.61689300	0.98049600	2.43376600	H -6.59182200	-1.11262800	-2.37074300
C 2.58447700	1.61843100	0.11212400	C 1.35674600	-0.05314500	2.19298500
N 1.55804700	0.25854700	-2.02655900	N 2.56637400	-1.46090400	0.20530300
2W-cis + PhCCH-TS			2W-trans + PhCCH-TS		
N 1.26232400	-2.40790500	0.00000000	O 2.49573400	-2.99857700	0.00000000
O 2.05916200	-3.28730500	0.00000000	P -0.03370300	-0.52241000	2.41381500
W 0.08702700	-1.02829200	0.00000000	P -0.03370300	-0.52241000	-2.41381500
P -0.01979500	-0.53960900	2.41566000	C -1.10400600	1.01643900	2.46407200
P -0.01979500	-0.53960900	-2.41566000	C -1.10400600	1.01643900	-2.46407200
C -1.07381400	1.00630800	2.45772200	H -0.42484900	1.87331800	2.48009100
C -1.07381400	1.00630800	-2.45772200	H -0.42484900	1.87331800	-2.48009100
H -0.38351800	1.85412000	2.46120600	H -1.71320400	1.06948500	3.36858600
H -0.38351800	1.85412000	-2.46120600	H -1.71320400	1.06948500	-3.36858600
H -1.67117100	1.07162200	3.36904500	C -1.98261900	1.09598800	1.22599300
H -1.67117100	1.07162200	-3.36904500	C -1.98261900	1.09598800	-1.22599300
C -1.96672200	1.09244100	1.22908500	H -2.48606500	2.07054700	1.18673600
C -1.96672200	1.09244100	-1.22908500	H -2.48606500	2.07054700	-1.18673600
H -2.46432900	2.07017800	1.19698600	H -2.75099200	0.32041000	1.24040700
H -2.46432900	2.07017800	-1.19698600	H -2.75099200	0.32041000	-1.24040700
H -2.74012500	0.32199700	1.25134300	N -1.17713200	0.89684400	0.00000000
H -2.74012500	0.32199700	-1.25134300	C 1.49022500	0.09313000	-3.32770400
N -1.16885000	0.89375800	0.00000000	C 1.49022500	0.09313000	3.32770400
C 1.54691200	0.07192400	-3.25746100	H 1.77879500	0.93802600	-2.69188200
C 1.54691200	0.07192400	3.25746100	H 1.77879500	0.93802600	2.69188200
H 1.78085500	0.94005900	-2.63091400	C -0.88507500	-1.73638100	-3.56608700
H 1.78085500	0.94005900	2.63091400	C -0.88507500	-1.73638100	3.56608700
C -0.82282900	-1.71763700	-3.64112800	C -2.38577400	-1.82237400	-3.29389900
C -0.82282900	-1.71763700	3.64112800	C -2.38577400	-1.82237400	3.29389900
C -2.33714800	-1.79315500	-3.46235900	O -1.93923000	-3.25400600	0.00000000
C -2.33714800	-1.79315500	3.46235900	H -0.73712100	-1.34569700	4.57875400
C -1.48267700	-2.21859200	0.00000000	H -0.73712100	-1.34569700	-4.57875400
O -2.39793500	-2.94245000	0.00000000	C -0.24518300	-3.12009000	3.46190800
H -0.61151200	-1.31198500	4.63611700	C -0.24518300	-3.12009000	-3.46190800
H -0.61151200	-1.31198500	-4.63611700	H 0.82224100	-3.10866900	3.68314700
C -0.20038500	-3.10783800	3.52184600	H 0.82224100	-3.10866900	-3.68314700
C -0.20038500	-3.10783800	-3.52184600	H -0.37339700	-3.53013400	2.45891000
H 0.87386400	-3.10562400	3.70898900	H -0.37339700	-3.53013400	-2.45891000
H 0.87386400	-3.10562400	-3.70898900	H -0.72534900	-3.80133600	4.17082400
H -0.36099500	-3.51785700	2.52260600	H -0.72534900	-3.80133600	-4.17082400
H -0.36099500	-3.51785700	-2.52260600	C 2.64433900	-0.90512000	-3.31668000
H -0.66284000	-3.78537800	4.24573900	C 2.64433900	-0.90512000	3.31668000
H -0.66284000	-3.78537800	-4.24573900	H 2.46896300	-1.73338300	-4.00679000
C 2.70829100	-0.90971000	-3.12449000	H 2.46896300	-1.73338300	4.00679000
C 2.70829100	-0.90971000	3.12449000	H 2.81375200	-1.32136800	-2.32344500
H 2.58941300	-1.77251900	-3.78353700	H 2.81375200	-1.32136800	2.32344500
H 2.58941300	-1.77251900	3.78353700	H 3.56402200	-0.40766800	-3.63861400
H 2.81039900	-1.27627300	-2.10196800	H 3.56402200	-0.40766800	3.63861400
H 2.81039900	-1.27627300	2.10196800	C 1.21555300	0.61329700	-4.73646900
H 3.64365800	-0.41641200	-3.40531100	C 1.21555300	0.61329700	4.73646900
H 3.64365800	-0.41641200	3.40531100	H 0.40568400	1.34538800	-4.76732700
C 1.36547400	0.54315400	-4.69747900	H 0.40568400	1.34538800	4.76732700
C 1.36547400	0.54315400	4.69747900	H 0.96488800	-0.19819700	-5.42421900
H 0.53839700	1.24841000	-4.80975900	H 0.96488800	-0.19819700	5.42421900
H 0.53839700	1.24841000	4.80975900	H 2.11175700	1.10144500	-5.13109000
H 1.19086700	-0.29390200	-5.37800300	H 2.11175700	1.10144500	5.13109000

H 1.19086700	-0.29390200	5.37800300	H 1.38995500	0.42100800	0.00000000
H 2.27394000	1.04851300	-5.03911400	H -0.44602700	1.62180400	0.00000000
H 2.27394000	1.04851300	5.03911400	C 2.05240700	1.76750100	0.00000000
H 1.32979800	0.43573900	0.00000000	H -2.83694500	-2.54236900	-3.98307600
H -0.43357700	1.61475300	0.00000000	H -2.58664700	-2.17223100	-2.27990900
C 2.01569800	1.79627700	0.00000000	H -2.89652600	-0.86916300	-3.44505600
H -2.75415000	-2.48878900	-4.19667500	H -2.83694500	-2.54236900	3.98307600
H -2.60408000	-2.16549900	-2.47235200	H -2.89652600	-0.86916300	3.44505600
H -2.82887300	-0.83038100	-3.61656200	H -2.58664700	-2.17223100	2.27990900
H -2.75415000	-2.48878900	4.19667500	C 1.43075300	2.84509800	0.00000000
H -2.82887300	-0.83038100	3.61656200	C 0.65021600	4.01197400	0.00000000
H -2.60408000	-2.16549900	2.47235200	C 0.25380100	4.63080200	1.20742600
C 1.38973700	2.86940200	0.00000000	C 0.25380100	4.63080200	-1.20742600
C 0.62268500	4.04711100	0.00000000	C -0.51043900	5.78440900	1.19849700
C 0.23347200	4.66893500	1.20722800	H 0.57319000	4.19957200	2.14921800
C 0.23347200	4.66893500	-1.20722800	C -0.51043900	5.78440900	-1.19849700
C -0.51767200	5.83130400	1.19871400	H 0.57319000	4.19957200	-2.14921800
H 0.54632100	4.23262800	2.14887000	C -0.90652500	6.37093200	0.00000000
C -0.51767200	5.83130400	-1.19871400	H -0.79528200	6.23780900	2.14223900
H 0.54632100	4.23262800	-2.14887000	H -0.79528200	6.23780900	-2.14223900
C -0.90655500	6.42204400	0.00000000	H -1.50269300	7.27570600	0.00000000
H -0.79804600	6.28760200	2.14234700	H 3.05262200	1.37181000	0.00000000
H -0.79804600	6.28760200	-2.14234700	W 0.07191300	-1.01607500	0.00000000
H -1.49275200	7.33334700	0.00000000	C 1.58316200	-2.27790500	0.00000000
H 3.00984400	1.38796500	0.00000000	N -1.16003100	-2.34916100	0.00000000
2W-cis + PhCCH-TS-H_M transfer to Ph-C			2W-trans + PhCCH-TS-H_M transfer to Ph-C		
C -2.63118900	-0.55597900	0.00000000	O -0.29290000	3.21495900	0.00000000
O -3.78441100	-0.73416600	0.00000000	P 0.57993700	-0.23262100	2.41836700
P -0.57535200	0.21716800	2.42226400	P 0.57993700	-0.23262100	-2.41836700
P -0.57535200	0.21716800	-2.42226400	C 0.74758300	-2.09704200	2.45712300
C -0.75916400	2.07672100	2.45095500	C 0.74758300	-2.09704200	-2.45712300
C -0.75916400	2.07672100	-2.45095500	H -0.27068800	-2.49672600	2.44155000
H 0.25739800	2.47986800	2.42279600	H -0.27068800	-2.49672600	-2.44155000
H 0.25739800	2.47986800	-2.42279600	H 1.22976100	-2.45632300	3.36845600
H -1.23057400	2.43463300	3.36804100	H 1.22976100	-2.45632300	-3.36845600
H -1.23057400	2.43463300	-3.36804100	C 1.49041200	-2.58741800	1.22366500
C -1.51791900	2.56692400	1.22676800	C 1.49041200	-2.58741800	-1.22366500
C -1.51791900	2.56692400	-1.22676800	H 1.44815900	-3.68475400	1.17732200
H -1.48869600	3.66485200	1.18740900	H 1.44815900	-3.68475400	-1.17732200
H -1.48869600	3.66485200	-1.18740900	H 2.54323500	-2.29838300	1.25453300
H -2.56694200	2.26536300	1.26291200	H 2.54323500	-2.29838300	-1.25453300
H -2.56694200	2.26536300	-1.26291200	N 0.89382400	-2.01233200	0.00000000
N -0.91605400	2.00721600	0.00000000	C -1.03238600	0.00032700	-3.35434400
C 1.05997200	-0.00724500	-3.31936800	C -1.03238600	0.00032700	3.35434400
C 1.05997200	-0.00724500	3.31936800	H -1.73869600	-0.49331400	-2.67773500
H 1.74733300	0.48614300	-2.62383100	H -1.73869600	-0.49331400	2.67773500
H 1.74733300	0.48614300	2.62383100	C 1.93093300	0.41150900	-3.55488900
C -1.87099600	-0.45690400	-3.60942100	C 1.93093300	0.41150900	3.55488900
C -1.87099600	-0.45690400	3.60942100	C 3.26281600	-0.30121900	-3.32753900
C -3.20613000	0.27518100	-3.49641800	C 3.26281600	-0.30121900	3.32753900
C -3.20613000	0.27518100	3.49641800	O 3.60204000	1.09000500	0.00000000
N -0.28535400	-2.02663000	0.00000000	H 1.59186200	0.19865500	4.57483100
O 0.01119100	-3.17824200	0.00000000	H 1.59186200	0.19865500	-4.57483100
C -2.06775900	-1.95524900	3.37948900	C 2.10559700	1.92099800	3.38925700
C -2.06775900	-1.95524900	-3.37948900	C 2.10559700	1.92099800	-3.38925700
H -1.14400600	-2.52420400	3.48509500	H 1.18237800	2.47470100	3.55903100
H -1.14400600	-2.52420400	-3.48509500	H 1.18237800	2.47470100	-3.55903100
H -2.45509000	-2.14209300	2.37637600	H 2.45670600	2.16025000	2.38450100
H -2.45509000	-2.14209300	-2.37637600	H 2.45670600	2.16025000	-2.38450100
H -2.78868600	-2.34925400	4.10226500	H 2.85006500	2.28449100	4.10427900
H -2.78868600	-2.34925400	-4.10226500	H 2.85006500	2.28449100	-4.10427900
C 1.46798200	-1.47547900	-3.41714900	C -1.44294800	1.46590800	-3.47064600

C	1.46798200	-1.47547900	3.41714900	C	-1.44294800	1.46590800	3.47064600
H	0.89310100	-1.99909000	-4.18501900	H	-0.85330500	1.98668400	-4.22895700
H	0.89310100	-1.99909000	4.18501900	H	-0.85330500	1.98668400	4.22895700
H	1.33408300	-2.00237600	-2.47113500	H	-1.33200000	1.99870800	-2.52579500
H	1.33408300	-2.00237600	2.47113500	H	-1.33200000	1.99870800	2.52579500
H	2.52285900	-1.54877900	-3.69593900	H	-2.49156900	1.53220700	-3.77368700
H	2.52285900	-1.54877900	3.69593900	H	-2.49156900	1.53220700	3.77368700
C	1.15344600	0.68526200	-4.67645100	C	-1.08567500	-0.69661000	-4.71168800
C	1.15344600	0.68526200	4.67645100	C	-1.08567500	-0.69661000	4.71168800
H	0.90983800	1.74843600	-4.62567600	H	-0.84466000	-1.75957100	-4.65115900
H	0.90983800	1.74843600	4.62567600	H	-0.84466000	-1.75957100	4.65115900
H	0.49530500	0.22164300	-5.41596300	H	-0.40475400	-0.23447200	-5.43122200
H	0.49530500	0.22164300	5.41596300	H	-0.40475400	-0.23447200	5.43122200
H	2.17442700	0.60326400	-5.06160400	H	-2.09440000	-0.61434600	-5.12754400
H	2.17442700	0.60326400	5.06160400	H	-2.09440000	-0.61434600	5.12754400
H	1.07738600	0.45244100	0.00000000	H	-1.11828800	-0.38703800	0.00000000
H	0.08738300	2.31513900	0.00000000	H	-0.11566200	-2.30810100	0.00000000
C	2.32200300	1.56138100	0.00000000	C	-2.34373600	-1.51388600	0.00000000
C	3.43102200	0.61748600	0.00000000	C	-3.47145500	-0.59186500	0.00000000
C	3.28842800	-0.76847000	0.00000000	C	-3.35897100	0.79621800	0.00000000
C	4.40448900	-1.59476600	0.00000000	C	-4.49107700	1.60032600	0.00000000
C	5.68171700	-1.05095800	0.00000000	C	-5.75679300	1.03053600	0.00000000
C	4.72659600	1.15924500	0.00000000	C	-4.75602000	-1.15970500	0.00000000
C	5.83712000	0.33219000	0.00000000	C	-5.88319000	-0.35562000	0.00000000
H	2.28714800	-1.18265300	0.00000000	H	-2.36830000	1.23185900	0.00000000
H	4.26988500	-2.67073100	0.00000000	H	-4.37815900	2.67878400	0.00000000
H	6.55203700	-1.69790100	0.00000000	H	-6.64028400	1.65930500	0.00000000
H	4.84359300	2.23675200	0.00000000	H	-4.85123400	-2.23932500	0.00000000
H	6.83010500	0.76858400	0.00000000	H	-6.86691200	-0.81254100	0.00000000
H	-1.47206600	-0.29822200	4.61713000	H	4.01314300	0.10899500	-4.01004200
H	-1.47206600	-0.29822200	-4.61713000	H	3.62805100	-0.14347200	-2.31110300
H	-3.92146300	-0.16361500	-4.19844400	H	3.20562700	-1.37456900	-3.51901700
H	-3.92146300	-0.16361500	4.19844400	H	4.01314300	0.10899500	4.01004200
H	-3.63091500	0.17392600	-2.49614100	H	3.20562700	-1.37456900	3.51901700
H	-3.63091500	0.17392600	2.49614100	H	3.62805100	-0.14347200	2.31110300
H	-3.12844100	1.33734400	-3.73711900	C	-1.96258700	-2.69496400	0.00000000
H	-3.12844100	1.33734400	3.73711900	H	-2.11774100	-3.75282100	0.00000000
W	-0.68025600	-0.25748000	0.00000000	C	0.08843200	2.11533900	0.00000000
C	1.94948000	2.74324300	0.00000000	N	2.45604600	0.75420200	0.00000000
H	2.06152100	3.80557700	0.00000000	W	0.71344400	0.24516900	0.00000000
2W-cis + PhCCH-interm				2W-trans + PhCCH-interm			
O	-3.69336000	-0.93075200	0.00000000	N	-2.40915300	-0.79020000	0.00000000
P	-0.57122500	0.23477700	2.43425400	O	-3.54871600	-1.14223900	0.00000000
P	-0.57122500	0.23477700	-2.43425400	P	-0.56559500	0.24607400	2.42750900
C	-0.84265500	2.08271100	2.45091800	P	-0.56559500	0.24607400	-2.42750900
C	-0.84265500	2.08271100	-2.45091800	C	-0.82253200	2.09990400	2.45526000
H	0.15336800	2.53458800	2.41659300	C	-0.82253200	2.09990400	-2.45526000
H	0.15336800	2.53458800	-2.41659300	H	0.17522000	2.54862600	2.42795800
H	-1.32546300	2.42305200	3.36845500	H	0.17522000	2.54862600	-2.42795800
H	-1.32546300	2.42305200	-3.36845500	H	-1.31012500	2.44133700	3.37017900
C	-1.63308000	2.52549800	1.22993800	H	-1.31012500	2.44133700	-3.37017900
C	-1.63308000	2.52549800	-1.22993800	C	-1.60467300	2.54544900	1.22949400
H	-1.67207200	3.62220700	1.18734200	C	-1.60467300	2.54544900	-1.22949400
H	-1.67207200	3.62220700	-1.18734200	H	-1.63219000	3.64243800	1.18233700
H	-2.65990200	2.15688600	1.26512400	H	-1.63219000	3.64243800	-1.18233700
H	-2.65990200	2.15688600	-1.26512400	H	-2.63547500	2.18779100	1.26375800
N	-0.99901600	2.00180500	0.00000000	H	-2.63547500	2.18779100	-1.26375800
C	1.07095500	0.08691400	-3.33233400	N	-0.97949100	2.00807800	0.00000000
C	1.07095500	0.08691400	3.33233400	C	1.06196200	0.08463000	-3.34914100
H	1.74491200	0.59655700	-2.63507500	C	1.06196200	0.08463000	3.34914100
H	1.74491200	0.59655700	2.63507500	H	1.74996800	0.59144000	-2.66333900
C	-1.84176700	-0.50200200	-3.60838600	H	1.74996800	0.59144000	2.66333900

C -1.84176700	-0.50200200	3.60838600	C -1.88004300	-0.46858700	-3.56343700
C -3.20768700	0.17086800	-3.49675300	C -1.88004300	-0.46858700	3.56343700
C -3.20768700	0.17086800	3.49675300	C -3.24236300	0.19389000	-3.36734100
O 0.10599200	-3.14737500	0.00000000	C -3.24236300	0.19389000	3.36734100
H -1.45000400	-0.32769400	4.61626000	C -0.06220200	-2.11023400	0.00000000
H -1.45000400	-0.32769400	-4.61626000	O 0.29099400	-3.21654100	0.00000000
C -1.96958100	-2.00739700	3.37648600	H -1.53372500	-0.25759400	4.58113700
C -1.96958100	-2.00739700	-3.37648600	H -1.53372500	-0.25759400	-4.58113700
H -1.01815900	-2.53149500	3.46594600	C -1.99483500	-1.98155700	3.37824700
H -1.01815900	-2.53149500	-3.46594600	C -1.99483500	-1.98155700	-3.37824700
H -2.36647000	-2.21211300	2.38088500	H -1.04467100	-2.49782600	3.51294000
H -2.36647000	-2.21211300	-2.38088500	H -1.04467100	-2.49782600	-3.51294000
H -2.65840800	-2.43599400	4.11048800	H -2.36569500	-2.22206300	2.38098500
H -2.65840800	-2.43599400	-4.11048800	H -2.36569500	-2.22206300	-2.38098500
C 1.53282900	-1.36297800	-3.45962300	H -2.70204200	-2.38606700	4.10858500
C 1.53282900	-1.36297800	3.45962300	H -2.70204200	-2.38606700	-4.10858500
H 0.97210000	-1.89495200	-4.23226100	C 1.51862200	-1.36523300	-3.48950900
H 0.97210000	-1.89495200	4.23226100	C 1.51862200	-1.36523300	3.48950900
H 1.43243500	-1.91177800	-2.52215500	H 0.94790800	-1.89158100	-4.25850000
H 1.43243500	-1.91177800	2.52215500	H 0.94790800	-1.89158100	4.25850000
H 2.58720400	-1.38801400	-3.74675100	H 1.42730700	-1.91844000	-2.55424500
H 2.58720400	-1.38801400	3.74675100	H 1.42730700	-1.91844000	2.55424500
C 1.12664500	0.80589600	-4.67784200	H 2.56944700	-1.39002100	-3.78933300
C 1.12664500	0.80589600	4.67784200	H 2.56944700	-1.39002100	3.78933300
H 0.85260100	1.86010400	-4.60588800	C 1.09509200	0.80669100	-4.69405800
H 0.85260100	1.86010400	4.60588800	C 1.09509200	0.80669100	4.69405800
H 0.47704800	0.33436700	-5.42000200	H 0.82881000	1.86213000	-4.61488100
H 0.47704800	0.33436700	5.42000200	H 0.82881000	1.86213000	4.61488100
H 2.14643400	0.76273300	-5.07116600	H 0.42778600	0.33972800	-5.42325300
H 2.14643400	0.76273300	5.07116600	H 0.42778600	0.33972800	5.42325300
H 1.17548600	0.71933500	0.00000000	H 2.10650700	0.75797700	-5.10756900
H -0.02792600	2.36507000	0.00000000	H 2.10650700	0.75797700	5.10756900
C 2.15904900	1.46968500	0.00000000	H 1.21333900	0.67467500	0.00000000
C 3.34491000	0.58876500	0.00000000	H -0.00234100	2.35122000	0.00000000
C 3.23419700	-0.80022900	0.00000000	C 2.19056600	1.44253800	0.00000000
C 4.36271000	-1.61172800	0.00000000	C 3.38667700	0.57423800	0.00000000
C 5.62902300	-1.04417900	0.00000000	C 3.29530200	-0.81545200	0.00000000
C 4.62905900	1.15097800	0.00000000	C 4.43329600	-1.61344100	0.00000000
C 5.75354900	0.34378100	0.00000000	C 5.69224100	-1.02997800	0.00000000
H 2.24470100	-1.24604800	0.00000000	C 4.66393700	1.15235400	0.00000000
H 4.24716500	-2.69028200	0.00000000	C 5.79853100	0.35953600	0.00000000
H 6.51218900	-1.67376600	0.00000000	H 2.31233600	-1.27330700	0.00000000
H 4.70708800	2.23226600	0.00000000	H 4.33105000	-2.69335800	0.00000000
H 6.73871400	0.79870600	0.00000000	H 6.58339000	-1.64816600	0.00000000
H -3.90149500	-0.30004400	-4.19926500	H 4.72776100	2.23454900	0.00000000
H -3.62996700	0.05139200	-2.49733300	H 6.77771200	0.82720300	0.00000000
H -3.17706700	1.23494900	-3.73907800	H -3.96325200	-0.25492800	-4.05694600
H -3.90149500	-0.30004400	4.19926500	H -3.62039800	0.03450700	-2.35577000
H -3.17706700	1.23494900	3.73907800	H -3.22543200	1.26590800	-3.57299700
H -3.62996700	0.05139200	2.49733300	H -3.96325200	-0.25492800	4.05694600
C 2.11304000	2.76693900	0.00000000	H -3.22543200	1.26590800	3.57299700
H 1.28966700	3.47632500	0.00000000	H -3.62039800	0.03450700	2.35577000
N -0.20475300	-2.00428900	0.00000000	C 2.13921800	2.73950200	0.00000000
C -2.55666300	-0.66740300	0.00000000	H 1.31284400	3.44462600	0.00000000
W -0.65514000	-0.24737500	0.00000000	W -0.69873000	-0.24105300	0.00000000
2W-cis + PhCCH-TS-H_N transfer to C-H			2W-trans + PhCCH-TS-H_N transfer to C-H		
N -0.96005900	2.00633200	0.00000000	N -2.42898700	-0.77354100	0.00000000
H 1.10793000	0.58506100	0.00000000	O -3.57305100	-1.11408000	0.00000000
H 0.02587800	2.32767300	0.00000000	P -0.56806000	0.23753800	2.42103400
C 2.21323900	1.51943100	0.00000000	P -0.56806000	0.23753800	-2.42103400
C 3.36613300	0.60675300	0.00000000	C -0.79122100	2.09723200	2.45599500
C 3.23720200	-0.77991900	0.00000000	C -0.79122100	2.09723200	-2.45599500

C	4.35874100	-1.60006600	0.00000000	H	0.21477100	2.52737000	2.43597800
C	5.63107700	-1.04568500	0.00000000	H	0.21477100	2.52737000	-2.43597800
C	5.77281100	0.33978600	0.00000000	H	-1.27728900	2.44411600	3.36984100
C	4.65580400	1.15766200	0.00000000	H	-1.27728900	2.44411600	-3.36984100
P	-0.56833000	0.22340000	2.42619600	C	-1.55914500	2.56297800	1.22843000
P	-0.56833000	0.22340000	-2.42619600	C	-1.55914500	2.56297800	-1.22843000
N	-0.23273600	-2.01533800	0.00000000	H	-1.56240700	3.66103700	1.18388500
C	-2.59469400	-0.60791300	0.00000000	H	-1.56240700	3.66103700	-1.18388500
C	1.06929000	0.04311100	-3.32856900	H	-2.59834400	2.22995000	1.26136500
C	1.06929000	0.04311100	3.32856900	H	-2.59834400	2.22995000	-1.26136500
C	-1.84991500	-0.48497100	-3.60810500	N	-0.94720700	2.01253300	0.00000000
C	-1.84991500	-0.48497100	3.60810500	C	1.05202900	0.05069900	-3.35276800
O	-3.74101500	-0.82619500	0.00000000	C	1.05202900	0.05069900	3.35276800
C	-0.80139900	2.07795600	2.45097000	H	1.74844700	0.55111200	-2.67098600
C	-0.80139900	2.07795600	-2.45097000	H	1.74844700	0.55111200	2.67098600
H	0.20421800	2.50815800	2.42206600	C	-1.89728100	-0.44779000	-3.55917300
H	0.20421800	2.50815800	-2.42206600	C	-1.89728100	-0.44779000	3.55917300
H	-1.27986000	2.42483400	3.36848300	C	-3.24785600	0.23478600	-3.35080900
H	-1.27986000	2.42483400	-3.36848300	C	-3.24785600	0.23478600	3.35080900
C	-1.57805600	2.54474700	1.22939600	C	-0.06681500	-2.11304900	0.00000000
C	-1.57805600	2.54474700	-1.22939600	O	0.30038600	-3.21634300	0.00000000
H	-1.58861300	3.64291600	1.19057200	H	-1.55406500	-0.23688400	4.57803500
H	-1.58861300	3.64291600	-1.19057200	H	-1.55406500	-0.23688400	-4.57803500
H	-2.61487400	2.20469300	1.26475500	C	-2.03652500	-1.95950800	3.38057500
H	-2.61487400	2.20469300	-1.26475500	C	-2.03652500	-1.95950800	-3.38057500
H	1.75113500	0.54398600	-2.63293200	H	-1.09742500	-2.49160500	3.53091500
H	1.75113500	0.54398600	2.63293200	H	-1.09742500	-2.49160500	-3.53091500
C	-3.20179800	0.21612300	-3.49888100	H	-2.39689200	-2.19798800	2.37894600
C	-3.20179800	0.21612300	3.49888100	H	-2.39689200	-2.19798800	-2.37894600
O	0.07692600	-3.16195100	0.00000000	H	-2.76083800	-2.34813500	4.10289800
H	-1.45381800	-0.32089300	4.61603200	H	-2.76083800	-2.34813500	-4.10289800
H	-1.45381800	-0.32089300	-4.61603200	C	1.49072800	-1.40539600	-3.48602600
C	-2.01094400	-1.98675200	3.37300000	C	1.49072800	-1.40539600	3.48602600
C	-2.01094400	-1.98675200	-3.37300000	H	0.91149600	-1.92859000	-4.25075000
H	-1.07265400	-2.53295700	3.46962600	H	0.91149600	-1.92859000	4.25075000
H	-1.07265400	-2.53295700	-3.46962600	H	1.39242600	-1.95188900	-2.54757200
H	-2.40173800	-2.17961200	2.37250000	H	1.39242600	-1.95188900	2.54757200
H	-2.40173800	-2.17961200	-2.37250000	H	2.54045900	-1.44633100	-3.78878300
H	-2.71637000	-2.40100800	4.09961700	H	2.54045900	-1.44633100	3.78878300
H	-2.71637000	-2.40100800	-4.09961700	C	1.09169900	0.76389100	-4.70217300
C	1.50623300	-1.41547800	-3.44447600	C	1.09169900	0.76389100	4.70217300
C	1.50623300	-1.41547800	3.44447600	H	0.83474100	1.82224700	-4.62963600
H	0.93712200	-1.94283900	-4.21412500	H	0.83474100	1.82224700	4.62963600
H	0.93712200	-1.94283900	4.21412500	H	0.41833300	0.29905600	-5.42708400
H	1.39174700	-1.95501600	-2.50316800	H	0.41833300	0.29905600	5.42708400
H	1.39174700	-1.95501600	2.50316800	H	2.10165300	0.70269900	-5.11813300
H	2.56048400	-1.46294700	-3.73024100	H	2.10165300	0.70269900	5.11813300
H	2.56048400	-1.46294700	3.73024100	H	1.14786600	0.54221100	0.00000000
C	1.14050000	0.75112500	-4.67906400	H	0.04150000	2.31687400	0.00000000
C	1.14050000	0.75112500	4.67906400	C	2.24443100	1.48589400	0.00000000
H	0.88011900	1.80952400	-4.61582900	C	3.40934700	0.58771200	0.00000000
H	0.88011900	1.80952400	4.61582900	C	3.30091300	-0.80011900	0.00000000
H	0.48574800	0.28382000	-5.41929000	C	4.43234500	-1.60651600	0.00000000
H	0.48574800	0.28382000	5.41929000	C	5.69719500	-1.03571600	0.00000000
H	2.16032400	0.69056100	-5.07065800	C	4.69232300	1.15490300	0.00000000
H	2.16032400	0.69056100	5.07065800	C	5.81974300	0.35169000	0.00000000
H	2.24099700	-1.20781500	0.00000000	H	2.31198800	-1.24147400	0.00000000
H	4.23250500	-2.67721100	0.00000000	H	4.31968200	-2.68519600	0.00000000
H	6.50717400	-1.68500700	0.00000000	H	6.58173400	-1.66325200	0.00000000
H	4.75247800	2.23720000	0.00000000	H	4.77385000	2.23560000	0.00000000
H	6.76237100	0.78444900	0.00000000	H	6.80320900	0.80972400	0.00000000
H	-3.90574100	-0.24223100	4.19978900	H	-3.98106900	-0.19969300	-4.03675100
H	-3.90574100	-0.24223100	-4.19978900	H	-3.62006600	0.07703600	-2.33684700

H -3.14918700	1.27877700	3.74416200	H -3.21550000	1.30737500	-3.55215400
H -3.14918700	1.27877700	-3.74416200	H -3.98106900	-0.19969300	4.03675100
H -3.62559100	0.10849400	2.49878900	H -3.21550000	1.30737500	3.55215400
H -3.62559100	0.10849400	-2.49878900	H -3.62006600	0.07703600	2.33684700
C 2.04726400	2.76646500	0.00000000	C 2.08968500	2.73801100	0.00000000
H 1.51284800	3.69160600	0.00000000	H 1.48559500	3.62170900	0.00000000
W -0.66172000	-0.25399500	0.00000000	W -0.69932400	-0.24423300	0.00000000
2W-cis + PhCHCH₂-TS-H_M transfer			2W-trans + PhCHCH₂-TS-H_M transfer		
O -2.27363700	2.28870700	-1.97627400	O -2.41103700	2.46315500	-1.49645000
P 1.31240000	1.86486800	-0.04896400	P 1.33056100	1.85240300	-0.06826500
P -2.31918400	-1.36141200	-0.09125500	P -2.31564500	-1.35470200	-0.10167200
C 2.30320700	0.82326000	-1.24144400	C 2.31839300	0.81129900	-1.26840900
C -1.43184700	-2.42096100	-1.35239500	C -1.44577600	-2.42011100	-1.37560000
H 2.92682100	0.15417200	-0.64236200	H 2.95191200	0.14623200	-0.67470100
H -0.86513300	-3.16823200	-0.79067300	H -0.89117200	-3.18520100	-0.82567200
H 2.97611500	1.42789900	-1.85272700	H 2.98076900	1.41599700	-1.89152400
H -2.12735900	-2.96178400	-1.99707100	H -2.14894300	-2.93927500	-2.03014300
C 1.38734000	-0.00258400	-2.13182300	C 1.39302000	-0.01997100	-2.14218600
C -0.47509400	-1.58626800	-2.19044600	C -0.47753900	-1.58500500	-2.19877000
H 1.98449900	-0.71157200	-2.71883700	H 1.98261900	-0.73917200	-2.72449500
H 0.15129500	-2.24458500	-2.80690300	H 0.14895100	-2.24194600	-2.81656500
H 0.84283100	0.63587100	-2.83087200	H 0.84739900	0.61290500	-2.84530400
H -1.02420200	-0.92453000	-2.86337900	H -1.01760200	-0.91422500	-2.87009300
N 0.38262200	-0.74042100	-1.33058600	N 0.38223000	-0.74390500	-1.33297100
C -2.50817700	-2.58272400	1.33019600	C -2.56531300	-2.61367500	1.27638300
C 2.46821900	1.94566600	1.43170700	C 2.53895300	1.98823400	1.36623600
H -1.47560700	-2.93106900	1.43874100	H -1.53745700	-2.95916200	1.43181600
H 2.62570900	0.87861000	1.61691500	H 2.66284900	0.93244300	1.62755100
C -4.06012600	-1.14043500	-0.76851700	C -4.02213900	-1.04809600	-0.82435900
C 1.32625800	3.60055300	-0.77400100	C 1.26934300	3.56232300	-0.84380800
C -4.07157200	-0.78364100	-2.25290800	C -3.95748500	-0.61020000	-2.28632800
C 1.05337400	3.60957300	-2.27635400	C 0.90781000	3.50872400	-2.32705500
O -2.08485300	1.98157000	2.44719400	O -1.82707400	1.74270000	2.83867200
H 2.33828300	3.98416600	-0.60824700	H 2.28428300	3.96384600	-0.75148900
H -4.55350300	-2.10994800	-0.64645900	H -4.54029000	-2.01168600	-0.77689700
C 0.32664500	4.49424500	-0.04143900	C 0.30069100	4.47327900	-0.09026400
C -4.81409900	-0.08968700	0.04481500	C -4.79100600	-0.02502700	0.01029500
H 0.52946500	4.56438300	1.02757300	H 0.54264000	4.56197100	0.96873100
H -4.89029400	-0.35099200	1.10096800	H -4.89373400	-0.32521300	1.05348300
H -0.69063200	4.11703000	-0.16085200	H -0.72236300	4.10404100	-0.16986600
H -4.31774500	0.88045300	-0.02084000	H -4.29419000	0.94585900	-0.01086500
H 0.36322000	5.50688700	-0.45401700	H 0.33131500	5.47755000	-0.52371200
H -5.83060300	0.02182900	-0.34388800	H -5.79744400	0.10098700	-0.39991300
C -2.90170900	-1.90245900	2.63879800	C -3.04415900	-1.98931100	2.58381800
C 1.79994700	2.53182900	2.67262900	C 1.95638100	2.70016100	2.58396100
H -3.94876100	-1.59229400	2.63532500	H -4.09568500	-1.69956600	2.53137600
H 1.68046700	3.61457900	2.59504800	H 1.90825500	3.78063300	2.43264300
H -2.29086500	-1.01953400	2.83374400	H -2.46492100	-1.10450300	2.84908800
H 0.81647000	2.09372800	2.84832500	H 0.95445400	2.34501000	2.82609500
H -2.77450200	-2.59847500	3.47334100	H -2.95061500	-2.71569900	3.39653700
H 2.42083800	2.33985200	3.55284900	H 2.59754800	2.52675800	3.45327400
C -3.38536800	-3.79589200	1.03331000	C -3.41375700	-3.82150100	0.88600800
C 3.82469200	2.58888200	1.15865100	C 3.90704500	2.55107400	0.98935000
H -3.12122100	-4.28728100	0.09366600	H -3.08386200	-4.28638700	-0.04576900
H 4.31912600	2.16975300	0.27953500	H 4.36098200	2.02616300	0.14671500
H -4.44369300	-3.52805300	0.98993100	H -4.46770100	-3.55474500	0.77799600
H 3.73916100	3.66932500	1.01999700	H 3.85163700	3.61382700	0.74093800
H -3.27565900	-4.53636300	1.83137500	H -3.35509500	-4.58280300	1.66953900
H 4.48831700	2.42924800	2.01393500	H 4.59055400	2.45745300	1.83862300
H 0.34247700	-0.64716000	1.22333700	H 0.33914400	-0.64640700	1.28127300
H 0.90257800	-1.38382800	-0.70409100	H 0.89742800	-1.39257000	-0.70610400
C 1.11689900	-1.77814100	1.76697300	C 1.07507000	-1.77134900	1.79029500

H -5.10740200	-0.68616000	-2.59147700	H -4.97413800	-0.45573100	-2.65983300
H -3.57674700	0.16925400	-2.44193200	H -3.42265100	0.33358700	-2.39877000
H -3.60231800	-1.54935700	-2.87418300	H -3.49015100	-1.35904900	-2.92910500
H 1.08061400	4.64047800	-2.64178100	H 0.88384000	4.52605300	-2.72877300
H 1.79866100	3.04807300	-2.84324200	H 1.63500700	2.94704200	-2.91672600
H 0.06497300	3.21029300	-2.50682300	H -0.08188100	3.07581300	-2.48114900
H 0.27242000	-2.13739000	2.34283000	H 0.23229500	-2.13318800	2.36899700
C 1.69334500	-2.64536300	0.84079300	C 1.64378200	-2.64555600	0.85931900
H 1.09323300	-3.47997700	0.48635600	H 1.03430900	-3.47253500	0.50346100
N -1.57742700	1.43296200	1.52639700	W -0.76475600	0.55877300	0.14123000
W -0.77522400	0.55568400	0.15725800	C -1.44282100	1.31601600	1.82802000
C -1.70793700	1.62453500	-1.20096200	N -1.75265800	1.68829400	-0.86979400
H 1.76383700	-1.13646100	2.35786400	H 1.73590300	-1.15582300	2.39503600
C 3.05187500	-2.61398100	0.35014800	C 3.00143700	-2.62716600	0.37226500
C 3.45115500	-3.50635200	-0.66810700	C 3.39890200	-3.53209500	-0.63708800
C 4.04931400	-1.75109400	0.84991900	C 4.00364400	-1.76322900	0.86299200
C 4.74492200	-3.52612000	-1.15908300	C 4.69317300	-3.56394100	-1.12503800
H 2.71804100	-4.20118100	-1.06798200	H 2.66311100	-4.22765000	-1.03086000
C 5.34331500	-1.77094500	0.35304700	C 5.29864000	-1.79649300	0.36926800
H 3.81492000	-1.07597700	1.66542600	H 3.77182500	-1.07686300	1.66987400
C 5.70699600	-2.65192400	-0.66021000	C 5.65996000	-2.69014900	-0.63364400
H 5.00838200	-4.23223300	-1.94009200	H 4.95388800	-4.27974400	-1.89819100
H 6.08311500	-1.09665900	0.77285100	H 6.04122400	-1.12153700	0.78321500
H 6.72080400	-2.66709800	-1.04283700	H 6.67436500	-2.71514500	-1.01407700
2W-cis + PhCHCH₂-interm			2W-trans + PhCHCH₂-interm		
O -2.34227100	2.32827100	-1.83717600	O -2.43469000	2.46356100	-1.44495300
P 1.30751900	1.86496700	-0.06982800	P 1.32856500	1.84598700	-0.07894300
P -2.34566000	-1.37044400	-0.08741100	P -2.33606800	-1.36239000	-0.09582400
C 2.29786200	0.80130500	-1.23647200	C 2.31611300	0.78599900	-1.25752200
C -1.44700900	-2.44369600	-1.32260100	C -1.45958100	-2.43850200	-1.35145200
H 2.91942700	0.14324900	-0.62258400	H 2.94637600	0.12803100	-0.65211200
H -0.89161600	-3.18542200	-0.74341200	H -0.91404200	-3.20150900	-0.79047600
H 2.97253200	1.39226900	-1.85890000	H 2.98163000	1.38054700	-1.88693800
H -2.13467900	-2.98827800	-1.97245500	H -2.15937800	-2.95820000	-2.00917100
C 1.38056900	-0.04353600	-2.10578000	C 1.39126800	-0.05750600	-2.11917700
C -0.47191100	-1.62092400	-2.15057900	C -0.47769700	-1.61379600	-2.16877500
H 1.97873900	-0.77623800	-2.66122800	H 1.98244200	-0.79487800	-2.67602100
H 0.17392000	-2.29253000	-2.73131300	H 0.16086800	-2.28168000	-2.76161600
H 0.84921300	0.57471100	-2.83302800	H 0.85863400	0.56112200	-2.84483300
H -1.00432500	-0.98052700	-2.85704400	H -1.00553000	-0.95727300	-2.86369900
N 0.36778000	-0.75634000	-1.28774500	N 0.37063100	-0.76053300	-1.30134000
C -2.56731900	-2.57362400	1.34343800	C -2.60587900	-2.60470700	1.29325800
C 2.45666000	1.99020400	1.41170800	C 2.52586500	2.00996500	1.36108900
H -1.53294200	-2.89656200	1.50252900	H -1.58061400	-2.94878500	1.46813400
H 2.57138200	0.93237600	1.66815200	H 2.63469200	0.96191300	1.65813100
C -4.07147300	-1.12438600	-0.79104000	C -4.03204200	-1.04357200	-0.83577400
C 1.29174400	3.58384100	-0.83100700	C 1.25641500	3.54219300	-0.88162100
C -4.05235600	-0.78592800	-2.27991700	C -3.94795200	-0.61053600	-2.29826600
C 1.02839500	3.55305900	-2.33492500	C 0.89316800	3.46088000	-2.36318100
O -2.00447500	1.89759000	2.53834800	O -1.79062700	1.70941300	2.86813200
H 2.29774400	3.98437800	-0.66767200	H 2.27151200	3.94543900	-0.79817100
H -4.58056300	-2.08546000	-0.66568500	H -4.55414100	-2.00523700	-0.79215900
C 0.27698300	4.48313200	-0.12631900	C 0.28950500	4.46707600	-0.14303200
C -4.82478500	-0.05424800	-0.00264500	C -4.80735700	-0.01667300	-0.01197400
H 0.45519200	4.56113500	0.94614500	H 0.53095700	4.57271600	0.91429800
H -4.91166600	-0.29550700	1.05716800	H -4.92270600	-0.31435800	1.03047600
H -0.73829800	4.10937200	-0.26701900	H -0.73496400	4.10137900	-0.21812700
H -4.32407600	0.91218200	-0.08226300	H -4.31020700	0.95394600	-0.03030500
H 0.32554300	5.49224200	-0.54616600	H 0.32400700	5.46391500	-0.59290800
H -5.83706000	0.05544800	-0.40253900	H -5.80884700	0.10962400	-0.43385600
C -3.03760400	-1.89297600	2.62640700	C -3.10564000	-1.96988700	2.58781800
C 1.81520500	2.68743300	2.60903100	C 1.94740600	2.77071000	2.55122200

H -4.09371200	-1.61997300	2.57561400	H -4.15710700	-1.68383600	2.51780600
H 1.76326400	3.76876300	2.46520700	H 1.92768400	3.84712200	2.36815900
H -2.46618200	-0.98901900	2.84206500	H -2.53267800	-1.08205600	2.85622900
H 0.80672200	2.32133100	2.80662000	H 0.93522600	2.44722000	2.79534900
H -2.92279200	-2.57740800	3.47201500	H -3.02190100	-2.68967000	3.40729500
H 2.41974100	2.51227000	3.50373200	H 2.57612100	2.60717300	3.43127300
C -3.40249500	-3.80939400	1.01879800	C -3.44803400	-3.81591700	0.89944500
C 3.83888900	2.55728600	1.10043600	C 3.90391300	2.54048800	0.97356400
H -3.07916000	-4.30791900	0.10202000	H -3.10167600	-4.29015400	-0.02142800
H 4.32614900	2.04284700	0.26989100	H 4.36017200	1.97227500	0.16117200
H -4.46251800	-3.56510400	0.91714400	H -4.49981400	-3.54987000	0.77058000
H 3.79591200	3.62387500	0.86667700	H 3.86349300	3.59181100	0.67783300
H -3.31860800	-4.53587100	1.83253200	H -3.40311200	-4.56923300	1.69141900
H 4.48622800	2.44858400	1.97576000	H 4.57692700	2.47642400	1.83371500
H 0.45612300	-0.76626900	1.27445600	H 0.42069300	-0.75085800	1.29891600
H 0.92279900	-1.43514400	-0.66600100	H 0.90384300	-1.43251100	-0.67435100
C 1.09766600	-1.72243500	1.66887400	C 1.05984300	-1.73717000	1.70664100
H -5.08049000	-0.67126000	-2.63573600	H -4.95941600	-0.45173700	-2.68362800
H -3.53573000	0.15479100	-2.47270600	H -3.40680200	0.32995400	-2.40809700
H -3.58893400	-1.56852400	-2.88389300	H -3.47723000	-1.36392700	-2.93296100
H 1.03627400	4.57567400	-2.72348100	H 0.86574200	4.47080200	-2.78275200
H 1.78794600	2.99367200	-2.88418600	H 1.62100700	2.89047900	-2.94325700
H 0.04926900	3.12868500	-2.56160900	H -0.09550500	3.02244200	-2.50859500
H 0.34610700	-2.22004700	2.28017300	H 0.28198500	-2.20337200	2.30894900
C 1.69036200	-2.54080000	0.63614200	C 1.64943100	-2.57652900	0.70247500
H 1.12996200	-3.41805300	0.32276700	H 1.07123100	-3.43435800	0.36916200
N -1.53375500	1.37861800	1.58287100	C 3.03148200	-2.57984700	0.31725100
W -0.77683900	0.53660100	0.16296500	C 3.49475600	-3.50117800	-0.65515200
C -1.74782100	1.64053700	-1.10512800	C 4.01114100	-1.71155800	0.85388500
H 1.80251900	-1.22066200	2.33291100	C 4.81441700	-3.54078200	-1.06169500
C 3.08177400	-2.55106200	0.28128700	H 2.78377400	-4.20185500	-1.08444300
C 3.56127100	-3.47677800	-0.67893900	C 5.33436200	-1.75584200	0.44005400
C 4.05335300	-1.68341300	0.83283000	H 3.73801300	-1.01230400	1.63681200
C 4.88748400	-3.51912700	-1.06256900	C 5.75601700	-2.66174000	-0.52653200
H 2.85688700	-4.17772100	-1.11857000	H 5.11878300	-4.26924500	-1.80705000
C 5.38368100	-1.73005000	0.44179600	H 6.05144500	-1.07629500	0.89082100
H 3.76838300	-0.98060600	1.60833600	H 6.79123100	-2.69406900	-0.84500200
C 5.82097000	-2.63919100	-0.51430300	H 1.75672900	-1.22436200	2.37017900
H 5.20388200	-4.25083600	-1.79971700	W -0.77285000	0.54981100	0.14228500
H 6.09344700	-1.04973700	0.90292300	C -1.42096200	1.28894300	1.84981800
H 6.86146100	-2.67367300	-0.81488200	N -1.77109900	1.68916400	-0.82465200
2W-cis + PhCHCH₂-TS-H_N transfer			2W-trans + PhCHCH₂-TS-H_N transfer		
O -2.40194700	2.34682900	-1.76320000	O -2.50353500	2.46986200	-1.34426900
P 1.29424200	1.87562100	-0.08513400	P 1.30465200	1.85753300	-0.09904500
P -2.34788500	-1.38337200	-0.08413700	P -2.34880700	-1.38061700	-0.08785700
C 2.29630000	0.80368500	-1.23036900	C 2.30610600	0.78482100	-1.24796100
C -1.42338000	-2.47744300	-1.27735000	C -1.42931700	-2.49172400	-1.27293600
H 2.92769900	0.16798600	-0.60377100	H 2.95182500	0.15865000	-0.62615900
H -0.87999300	-3.20569200	-0.67118000	H -0.89705000	-3.22785900	-0.66597800
H 2.96116800	1.39142100	-1.86646000	H 2.95632700	1.37486400	-1.89743600
H -2.09710200	-3.03618600	-1.93006600	H -2.10589200	-3.04128900	-1.93095200
C 1.38693000	-0.07374900	-2.07583400	C 1.39148100	-0.10390100	-2.07401600
C -0.43201600	-1.66667500	-2.09885200	C -0.42729600	-1.68739500	-2.08640700
H 1.99549200	-0.82798500	-2.59098500	H 1.99617600	-0.86799100	-2.57940400
H 0.24509200	-2.35253900	-2.62617800	H 0.25273800	-2.37709200	-2.60509000
H 0.87480900	0.51605500	-2.84105600	H 0.87803200	0.47448600	-2.84703200
H -0.95032800	-1.07323300	-2.85662200	H -0.93658100	-1.09528000	-2.85138900
N 0.36590900	-0.75651400	-1.24580600	N 0.36617600	-0.77033500	-1.23537400
C -2.59384400	-2.55166400	1.37135700	C -2.67442000	-2.57187600	1.33345400
C 2.43466100	2.03044700	1.40086600	C 2.49404700	2.06889900	1.34187200
H -1.56174700	-2.86945200	1.55504900	H -1.65292700	-2.87868600	1.58470800
H 2.57240200	0.97554200	1.65922000	H 2.62040100	1.02765900	1.65730600

C -4.05675600	-1.15913100	-0.83274100	C -4.01313000	-1.07789200	-0.90095900
C 1.26746500	3.57907000	-0.87750200	C 1.20892600	3.53025700	-0.94498800
C -3.99751500	-0.81704100	-2.31993000	C -3.86352300	-0.66259300	-2.36348600
C 0.97152700	3.51512400	-2.37443200	C 0.80892500	3.40087500	-2.41369000
O -1.96632200	1.84632600	2.58133700	O -1.73437200	1.62121200	2.92622500
H 2.27944400	3.97634100	-0.74578800	H 2.22669600	3.93323400	-0.90016100
H -4.55269300	-2.12939900	-0.72548600	H -4.53001100	-2.04315500	-0.86957300
C 0.27460000	4.50002100	-0.17017200	C 0.26323500	4.48103800	-0.21221400
C -4.85275100	-0.10493400	-0.06545000	C -4.83372500	-0.04730600	-0.12703900
H 0.48796300	4.61269700	0.89275100	H 0.53583800	4.62489700	0.83288100
H -4.97516200	-0.35545800	0.98861500	H -4.99721500	-0.33419100	0.91167000
H -0.74461500	4.12277900	-0.26608200	H -0.76339700	4.11542600	-0.24504000
H -4.36472700	0.86959200	-0.12089400	H -4.34569800	0.92776200	-0.13391900
H 0.30874200	5.49523000	-0.62323300	H 0.28496500	5.46106300	-0.69834100
H -5.85135600	-0.00699200	-0.50117300	H -5.81474700	0.06536500	-0.59809200
C -3.08650600	-1.84669400	2.63268300	C -3.27152100	-1.90531500	2.56984000
C 1.77895700	2.71475100	2.59798700	C 1.90535900	2.84007900	2.52027700
H -4.14176900	-1.57597500	2.55929000	H -4.33048200	-1.67750100	2.43223600
H 1.70456500	3.79469400	2.45441200	H 1.87631100	3.91368200	2.32305900
H -2.52006400	-0.93856000	2.84233100	H -2.75710200	-0.97972900	2.82804200
H 0.77834000	2.32897800	2.79679700	H 0.89593000	2.51111500	2.76748300
H -2.98555100	-2.51561000	3.49239200	H -3.19792100	-2.58375900	3.42474600
H 2.38761100	2.55227600	3.49233700	H 2.53367500	2.69418700	3.40370500
C -3.42236500	-3.79477900	1.05761500	C -3.45972500	-3.81993600	0.93693300
C 3.80475700	2.62646700	1.08953600	C 3.86314600	2.61516700	0.94410300
H -3.08065600	-4.31321200	0.15875600	H -3.03897300	-4.32487600	0.06498900
H 4.30109400	2.12497200	0.25639900	H 4.32788400	2.04093700	0.14083000
H -4.47999100	-3.55258700	0.92910400	H -4.50521700	-3.58547500	0.72303100
H 3.73872400	3.69257900	0.85901400	H 3.80419100	3.66042700	0.63043300
H -3.35520400	-4.50288600	1.88891100	H -3.45519300	-4.53657000	1.76349500
H 4.45555100	2.52872500	1.96357900	H 4.53785600	2.57720400	1.80446300
H 0.48054100	-0.77481800	1.34484700	H 0.47314000	-0.79417900	1.36765400
H 0.98244600	-1.47939200	-0.58164700	H 0.98313600	-1.49718900	-0.56112900
C 1.12478100	-1.71061400	1.64979700	C 1.10820700	-1.74318400	1.66128100
H -5.01596400	-0.71935500	-2.70727300	H -4.85614800	-0.50522700	-2.79546500
H -3.49122400	0.13266000	-2.49529200	H -3.31416800	0.27485800	-2.45995400
H -3.50152700	-1.59016500	-2.90990100	H -3.36637900	-1.42461700	-2.96665800
H 0.97726400	4.52836500	-2.78684600	H 0.77020800	4.39648900	-2.86528900
H 1.71593300	2.93775900	-2.92561600	H 1.52234600	2.81090500	-2.99179600
H -0.01405900	3.09095500	-2.57101000	H -0.18215100	2.95671200	-2.52004400
H 0.42096200	-2.28042200	2.25691300	H 0.38908000	-2.31670900	2.24678800
C 1.69057500	-2.44460900	0.51243300	C 1.68141700	-2.46031500	0.51841800
H 1.17353900	-3.36949300	0.26154300	H 1.17280800	-3.38738900	0.25852700
N -1.51611500	1.34761500	1.60528800	W -0.78539600	0.53595400	0.14317600
W -0.78073900	0.52850000	0.15759500	H 1.83277900	-1.31148200	2.35389500
C -1.78832800	1.65398800	-1.05276500	C 3.10606400	-2.50381300	0.24855300
H 1.85759500	-1.26338200	2.32339800	C 3.61257200	-3.42038300	-0.70126500
C 3.11221800	-2.50015900	0.23499500	C 4.05946100	-1.66300300	0.85916800
C 3.60673100	-3.42937200	-0.70942000	C 4.95529900	-3.48013700	-1.02345400
C 4.07620000	-1.66155700	0.83286500	H 2.91814900	-4.10135600	-1.18580200
C 4.94678900	-3.50161600	-1.03941200	C 5.40808100	-1.72453200	0.53222300
H 2.90441100	-4.10954200	-1.18360700	H 3.74819600	-0.96279700	1.62699300
C 5.42199600	-1.73564300	0.49770700	C 5.87456700	-2.62591500	-0.41546100
H 3.77556900	-0.95288900	1.59711500	H 5.29476200	-4.20542200	-1.75653300
C 5.87613600	-2.64852900	-0.44506900	H 6.10520900	-1.06224100	1.03655100
H 5.27638700	-4.23597300	-1.76796500	H 6.92770600	-2.67364100	-0.66655900
H 6.12705700	-1.07418600	0.99203500	N -1.82189500	1.69796600	-0.74138300
H 6.92727200	-2.70597300	-0.70240700	C -1.38993600	1.22798500	1.88850300
2W-cis + PhCHO-TS-H_M transfer			2W-trans + PhCHO-TS-H_M transfer		
O 2.20877200	3.09440600	-0.18126400	O 2.08757500	3.00448500	-0.65827700
P -1.57321300	1.64261100	0.18799800	P -1.59248600	1.61541600	0.21602400
P 2.53025000	-0.97812700	0.18342400	P 2.54397500	-0.94670300	0.19526800

C -1.74781700	1.37120600	2.02775400	C -1.77445800	1.33087100	2.05703300
C 2.50161600	-1.11627700	2.04722500	C 2.53248200	-1.08989700	2.06182100
H -2.29152000	0.42928400	2.14658400	H -2.32531800	0.39226500	2.17126600
H 1.96177400	-2.03767000	2.28150500	H 2.02476500	-2.02821000	2.30038900
H -2.33787400	2.15398600	2.50898400	H -2.35836500	2.11445000	2.54523300
H 3.50478400	-1.19906200	2.46955200	H 3.53980300	-1.13535800	2.48050800
C -0.38300200	1.24976500	2.69007600	C -0.40930700	1.19980800	2.71481700
C 1.75704300	0.05990600	2.66213400	C 1.75124400	0.06388400	2.67184600
H -0.50654800	0.98478900	3.74859900	H -0.53031200	0.90788400	3.76671700
H 1.62173900	-0.11175900	3.73837700	H 1.61327500	-0.11210500	3.74722200
H 0.15577100	2.19906800	2.64899800	H 0.12207700	2.15369300	2.69744400
H 2.31814300	0.98938100	2.54125500	H 2.28672300	1.00890600	2.55533700
N 0.43950800	0.22738900	2.01303400	N 0.43228300	0.20650600	2.01562200
C 2.52694200	-2.79407600	-0.31281400	C 2.61919800	-2.76474400	-0.28594200
C -3.18216200	0.93346500	-0.46365100	C -3.22519600	0.94524300	-0.42227300
H 1.66260300	-3.15939900	0.25109900	H 1.75774500	-3.16076700	0.26214500
H -3.09567000	-0.10890100	-0.14327800	H -3.14745000	-0.10832200	-0.13672300
C 4.25979400	-0.37690600	-0.25120700	C 4.23614500	-0.24581600	-0.22330100
C -1.73253400	3.50008800	-0.07175300	C -1.69720400	3.47871800	-0.00605600
C 4.74493100	0.74830500	0.65968900	C 4.60546600	0.94552700	0.65842200
C -0.99130400	4.31719800	0.98384100	C -0.85477400	4.23961800	1.01577000
O 0.52178400	0.39374600	-3.26468300	O 0.24264600	0.01311700	-3.33618800
H -2.80205300	3.71805300	0.01655100	H -2.74982700	3.73357900	0.15869800
H 4.91786900	-1.23914200	-0.10461300	H 4.94607400	-1.05431900	-0.02011500
C -1.26176700	3.88840000	-1.47328900	C -1.30291000	3.88543100	-1.42629600
C 4.32017100	0.05190600	-1.71635900	C 4.31969700	0.13186500	-1.70127300
H -1.79137900	3.35137600	-2.26011800	H -1.89124500	3.37746700	-2.18988500
H 4.04117100	-0.74982700	-2.40116100	H 4.10839100	-0.70913800	-2.36258100
H -0.19683500	3.68547300	-1.59496300	H -0.25103400	3.66928900	-1.61492900
H 3.64852500	0.89211400	-1.90188100	H 3.61335900	0.92865300	-1.93844500
H -1.42228000	4.95897900	-1.63302600	H -1.45276600	4.96224900	-1.55190500
H 5.33680300	0.36715300	-1.96966700	H 5.32684200	0.49169200	-1.93248100
C 2.23104800	-2.99246400	-1.79707300	C 2.37810400	-3.00166800	-1.77382700
C -3.24347000	0.93938200	-1.98929000	C -3.33848100	1.00114000	-1.94354500
H 3.08951100	-2.72921100	-2.41890300	H 3.24223900	-2.70979000	-2.37445600
H -3.42786800	1.94193400	-2.38265200	H -3.54148900	2.01526900	-2.29557900
H 1.38281300	-2.38743500	-2.12217100	H 1.51418300	-2.44448400	-2.13802400
H -2.32273200	0.55936500	-2.43473300	H -2.43369400	0.64157400	-2.43467600
H 1.99996800	-4.04346100	-1.99521600	H 2.20282000	-4.06602600	-1.95697300
H -4.06746000	0.30367100	-2.32458800	H -4.17158200	0.37270300	-2.26987400
C 3.74614300	-3.59521000	0.13605900	C 3.86251900	-3.50078900	0.20769400
C -4.44607500	1.52761600	0.15154700	C -4.46133100	1.53909800	0.24846600
H 3.97563100	-3.45276500	1.19468400	H 4.04810500	-3.34541400	1.27273000
H -4.43393200	1.50460200	1.24336700	H -4.42638800	1.46773300	1.33730000
H 4.63624500	-3.33758400	-0.44284700	H 4.75670900	-3.19729100	-0.34206000
H -4.60808600	2.56126400	-0.16497100	H -4.60495200	2.58913000	-0.01942600
H 3.56343500	-4.66311400	-0.01755100	H 3.74028100	-4.57677700	0.05142500
H -5.31666500	0.95197700	-0.17591500	H -5.35210400	0.99839400	-0.08408300
H -0.57988900	-1.08010800	-0.06021400	H -0.57249400	-1.10162900	-0.12766600
H -0.05032600	-0.68301100	2.11911300	H -0.03338000	-0.71870800	2.10355300
C -1.01696500	-2.46709000	0.81398900	C -0.94521500	-2.49283800	0.70782500
C -2.42918000	-2.59178200	0.33696600	C -2.37778500	-2.60806500	0.28643400
C -2.70329800	-2.87887800	-0.99943100	C -2.70869400	-2.85462700	-1.04507800
C -4.00963700	-3.07665400	-1.41980900	C -4.03204300	-3.03974300	-1.41560100
C -5.05483400	-2.99652800	-0.50376800	C -5.03755900	-2.98650600	-0.45441300
C -3.47719500	-2.52313000	1.25220600	C -3.38598200	-2.56694900	1.24662800
C -4.78601700	-2.72204100	0.83225600	C -4.71182800	-2.75250800	0.87666100
H -1.88519900	-2.92979400	-1.71131900	H -1.92218900	-2.88611700	-1.79290800
H -4.21650800	-3.29533800	-2.46162100	H -4.28273900	-3.22767600	-2.45378200
H -6.07629900	-3.15667800	-0.83114000	H -6.07218500	-3.13656300	-0.74289600
H -3.24146700	-2.33540100	2.29364300	H -3.10569900	-2.41156400	2.28234700
H -5.59803900	-2.67497300	1.54984600	H -5.49265200	-2.72686600	1.62913700
H 5.76032800	1.03379800	0.36847900	H 5.60477200	1.29748600	0.38496800

H 4.12024500	1.63735300	0.57110600	H 3.91705700	1.77915600	0.51628800
H 4.78357400	0.45248300	1.70999900	H 4.63457900	0.68931300	1.71933700
H -1.13265000	5.38305100	0.78090100	H -0.95430600	5.31431800	0.83629200
H -1.35738200	4.13087800	1.99546700	H -1.17168200	4.05422400	2.04404700
H 0.08229100	4.12416700	0.95794800	H 0.20420400	3.99271700	0.92138400
O -0.74991800	-2.27209200	2.01658500	O -0.63047100	-2.35257200	1.90815700
H -0.30672800	-3.00292500	0.16654700	H -0.26286300	-3.00753300	0.01298700
N 0.53825100	0.42943300	-2.07975300	C 0.36442200	0.19700600	-2.19532300
C 1.60274300	2.09733800	-0.20006700	N 1.49196400	1.98680300	-0.46899700
W 0.54197500	0.43849500	-0.26744400	W 0.54221100	0.45789300	-0.24980400
2W-cis + PhCHO-interm			2W-trans + PhCHO-interm		
O 2.20659500	3.04509800	-0.45456700	O 2.08053500	2.95956800	-0.77253500
P -1.57993000	1.66054600	0.20090300	P -1.60307700	1.62228700	0.22331700
P 2.54881300	-0.98227900	0.19965500	P 2.55395200	-0.95525200	0.20760100
C -1.77748500	1.33822900	2.02412400	C -1.80336600	1.28815000	2.04779500
C 2.45959200	-1.17460500	2.05002000	C 2.50475300	-1.12801200	2.06477200
H -2.32920300	0.39709000	2.10564200	H -2.35503000	0.34662000	2.12666700
H 1.90021700	-2.09594800	2.23366500	H 1.98749000	-2.06817700	2.27262500
H -2.36379100	2.11384100	2.52129800	H -2.39125100	2.06033100	2.54912100
H 3.44726200	-1.27720800	2.50332800	H 3.50373300	-1.18078200	2.50213900
C -0.41996100	1.17281800	2.69064800	C -0.44590000	1.12755800	2.71393600
C 1.69366800	-0.01409900	2.66792100	C 1.70431600	0.01301100	2.67348600
H -0.56650200	0.82623700	3.72300600	H -0.58791400	0.76226700	3.74002500
H 1.49423700	-0.23909500	3.72453300	H 1.51880000	-0.20415400	3.73412900
H 0.10788700	2.12959700	2.74282100	H 0.07056800	2.08911300	2.78080900
H 2.28164400	0.90851200	2.63726300	H 2.25796800	0.95514000	2.62493500
N 0.41343900	0.19844500	1.96275600	N 0.41302100	0.18293900	1.97312600
C 2.55970100	-2.77587500	-0.36366100	C 2.63442000	-2.76043500	-0.31324400
C -3.18450100	0.98436200	-0.49609900	C -3.23153700	0.98311100	-0.45634200
H 1.65320600	-3.15077900	0.12338200	H 1.74407300	-3.15959400	0.18438100
H -3.13118800	-0.06187600	-0.17808300	H -3.17772500	-0.07592100	-0.18337900
C 4.27558200	-0.34052600	-0.17095200	C 4.23977000	-0.22853200	-0.18190800
C -1.69448900	3.52471500	-0.00746900	C -1.66970300	3.48966800	0.04108800
C 4.69734700	0.78432100	0.77137500	C 4.57672800	0.95941100	0.71731900
C -0.88953100	4.28515900	1.04365300	C -0.79666200	4.20675400	1.06870600
O 0.40006100	0.18977500	-3.23984700	O 0.19754600	-0.09066000	-3.31334700
H -2.75402600	3.76360100	0.13531200	H -2.71471700	3.75611300	0.23356400
H 4.94220500	-1.19256600	-0.00330700	H 4.95359200	-1.03145500	0.03040800
C -1.27647800	3.95016400	-1.41467200	C -1.29832000	3.92826400	-1.37555000
C 4.39153000	0.10122500	-1.62877000	C 4.35076100	0.15919200	-1.65555600
H -1.41643500	5.02898100	-1.52848300	H -1.90964200	3.44996100	-2.14000900
H 4.15297800	-0.69736800	-2.33199200	H 4.15562900	-0.67774200	-2.32640200
H -1.85610400	3.45679400	-2.19492200	H -0.25331500	3.70679300	-1.59312600
H 3.72203400	0.93752100	-1.83752900	H 3.65022600	0.95753800	-1.90355600
H -0.22375700	3.72917800	-1.59327300	H -1.43695300	5.00977800	-1.46815400
H 5.41517400	0.42967000	-1.83423500	H 5.36181300	0.52226500	-1.86297600
C 2.37465700	-2.93336600	-1.87099200	C 2.46634900	-2.97206400	-1.81492200
C -3.22539300	0.99674300	-2.02238900	C -3.32649900	1.06029600	-1.97789600
H 3.28279500	-2.67226000	-2.41902100	H 3.36583600	-2.68956900	-2.36604700
H -3.40329500	2.00076400	-2.41428400	H -3.53017800	2.07812500	-2.31818700
H 1.56139000	-2.31348600	-2.25147400	H 1.63092900	-2.39927500	-2.21853800
H -2.30236800	0.61610500	-2.46228000	H -2.41628400	0.71101700	-2.46633900
H 2.14514500	-3.97605300	-2.10814300	H 2.28240300	-4.03076100	-2.01939000
H -4.04684500	0.36393300	-2.36813100	H -4.15302500	0.43259900	-2.32123000
C 3.74004800	-3.59622900	0.14954600	C 3.84939400	-3.51095700	0.22741500
C -4.44510400	1.60074400	0.10418400	C -4.46697000	1.58539100	0.20871900
H 3.88184200	-3.49892200	1.22818000	H 3.97638100	-3.38490700	1.30453900
H -4.44841200	1.57305400	1.19571100	H -4.44615700	1.49607800	1.29635200
H 4.67394200	-3.31693800	-0.34447700	H 4.77226900	-3.19515000	-0.26526400
H -4.58349300	2.63784700	-0.21187100	H -4.59262900	2.64101600	-0.04593900
H 3.57072000	-4.65585300	-0.06264900	H 3.73402900	-4.58181800	0.03592900
H -5.32024300	1.04097800	-0.23711400	H -5.35997300	1.06100400	-0.14274400

H -0.71300900	-1.23521600	0.01355700	H -0.68399700	-1.22757400	-0.02448600
H -0.12585200	-0.80322000	2.03602900	H -0.07724800	-0.81924100	2.02774600
C -0.98502400	-2.21145200	0.67188100	C -0.92154200	-2.24940300	0.60897300
C -2.42384300	-2.50360900	0.27552700	C -2.37130600	-2.52555200	0.24015100
C -2.76932600	-2.75568400	-1.05178800	C -2.75021100	-2.74473000	-1.08346100
C -4.07785500	-3.06828300	-1.39268700	C -4.06938300	-3.03734800	-1.39963700
C -5.05758500	-3.13800100	-0.40608500	C -5.02592400	-3.11943100	-0.39153200
C -3.40417500	-2.58417600	1.25823900	C -3.32802900	-2.61997600	1.24456400
C -4.71652500	-2.89788000	0.91875700	C -4.65089600	-2.91311400	0.93007700
H -2.00761900	-2.70091400	-1.82438300	H -2.00644200	-2.68100800	-1.87306900
H -4.33586400	-3.26166000	-2.42826700	H -4.35366700	-3.20594400	-2.43286100
H -6.07917300	-3.38752600	-0.67048400	H -6.05618700	-3.35317900	-0.63700800
H -3.10550200	-2.41507600	2.28618900	H -3.00230900	-2.47940400	2.26903100
H -5.47282600	-2.96405500	1.69356600	H -5.38953700	-2.99107200	1.72107400
H 5.71581400	1.09776500	0.52377500	H 5.57577500	1.32749100	0.46559100
H 4.05490200	1.65945900	0.66850000	H 3.87969400	1.78513200	0.57003500
H 4.69991500	0.47527100	1.81834700	H 4.58798500	0.69351400	1.77588900
H -1.00527700	5.36022700	0.87911700	H -0.87290400	5.28711600	0.91428600
H -1.22464000	4.07569100	2.06113500	H -1.10598400	4.00411400	2.09565000
H 0.17565600	4.05970900	0.97373700	H 0.25501600	3.93674700	0.95739700
O -0.75054900	-2.03317600	1.96226400	O -0.64143100	-2.13279000	1.88892000
H -0.34725100	-2.96723400	0.17481200	H -0.29009300	-2.95815600	0.03842200
W 0.54206400	0.43241700	-0.25262500	N 1.47499800	1.95407200	-0.56177000
C 1.58661500	2.06114300	-0.37339000	C 0.33346100	0.12602200	-2.18084200
N 0.47229400	0.31298000	-2.06518000	W 0.54465200	0.45632200	-0.24522000
2W-cis + PhCHO-TS-H_N transfer			2W-trans + PhCHO-TS-H_N transfer		
O 2.22649600	3.03095500	-0.44078200	O 2.12369500	2.92506400	-0.82369700
P -1.57045800	1.66952900	0.20726400	P -1.57651400	1.65083000	0.22099100
P 2.54077100	-1.00123000	0.20252300	P 2.54767600	-0.98171300	0.20885000
C -1.77534300	1.33935700	2.02784300	C -1.79436300	1.30933100	2.04061500
C 2.44554500	-1.20325900	2.05144200	C 2.46432200	-1.19593300	2.05920800
H -2.33605700	0.40318900	2.10319000	H -2.37071600	0.38219300	2.11046900
H 1.88361000	-2.12402200	2.22847400	H 1.93170800	-2.13332800	2.23901100
H -2.35522900	2.11794000	2.52810400	H -2.36386400	2.09393600	2.54394700
H 3.43173100	-1.31136100	2.50702400	H 3.45530800	-1.27335600	2.51121500
C -0.42065000	1.15710400	2.69598700	C -0.44379200	1.10677700	2.70937800
C 1.68142500	-0.04301000	2.67263000	C 1.66955600	-0.05643000	2.67854600
H -0.57334600	0.80146200	3.72418600	H -0.60235100	0.71850100	3.72501300
H 1.47412600	-0.27629700	3.72597500	H 1.45211300	-0.30300000	3.72699700
H 0.11307400	2.11053900	2.76085500	H 0.08673300	2.05891600	2.80880100
H 2.27718000	0.87516300	2.65563400	H 2.24863300	0.87257700	2.67829400
N 0.40790700	0.18400100	1.96116000	N 0.40131400	0.16333900	1.95322400
C 2.53997700	-2.79210200	-0.37039100	C 2.62201000	-2.77441500	-0.35600600
C -3.17787000	1.00701500	-0.49663800	C -3.21016400	1.03944200	-0.47312800
H 1.63012500	-3.16276900	0.11312100	H 1.70917700	-3.17345800	0.09964900
H -3.13269900	-0.04080700	-0.18268800	H -3.18033800	-0.01810000	-0.18992900
C 4.27248500	-0.36975000	-0.16160500	C 4.24510900	-0.25939200	-0.13406600
C -1.67201800	3.53524000	0.00660200	C -1.60900700	3.51994200	0.05284700
C 4.69874500	0.74897700	0.78639500	C 4.56390700	0.91561000	0.78849600
C -0.86274500	4.28453000	1.06259500	C -0.70659700	4.20747000	1.07538800
O 0.40291700	0.19500200	-3.23495500	O 0.17590900	-0.14233700	-3.29793400
H -2.72965700	3.78073700	0.14953500	H -2.64548000	3.80549200	0.26342300
H 4.93352900	-1.22645800	0.00478800	H 4.95008800	-1.06825400	0.08574200
C -1.24970600	3.96391700	-1.39818900	C -1.24929900	3.96467100	-1.36467200
C 4.39543600	0.07696500	-1.61745700	C 4.39472000	0.14676400	-1.59942000
H -1.38164900	5.04459500	-1.50695000	H -1.88823900	3.51434200	-2.12355300
H 4.15368500	-0.71770800	-2.32374700	H 4.21150200	-0.67991100	-2.28590800
H -1.83231300	3.47859000	-2.18087100	H -0.21522000	3.71570700	-1.60378100
H 3.73148100	0.91761100	-1.82503200	H 3.70688100	0.95364200	-1.85472200
H -0.19820400	3.73600500	-1.57688300	H -1.35761000	5.05081900	-1.44198200
H 5.42113800	0.39976700	-1.81887900	H 5.41313400	0.50545700	-1.77630400
C 2.35697200	-2.94136600	-1.87864300	C 2.50274700	-2.94972100	-1.86717800

C	-3.21554800	1.02571500	-2.02293200	C	-3.28984000	1.10344700	-1.99608900
H	3.26780100	-2.68426200	-2.42359000	H	3.42802800	-2.67747500	-2.37923500
H	-3.38596500	2.03246300	-2.41113800	H	-3.47300000	2.12102900	-2.34820000
H	1.54908500	-2.31398300	-2.25803700	H	1.69550800	-2.35018300	-2.28847100
H	-2.29436600	0.64106700	-2.46276400	H	-2.38129800	0.73438300	-2.47260300
H	2.12030600	-3.98152000	-2.12082200	H	2.30306700	-3.99949200	-2.10091400
H	-4.04067400	0.39986900	-2.37307600	H	-4.12379700	0.48662100	-2.34129200
C	3.71384700	-3.62297200	0.14155300	C	3.80753800	-3.55510500	0.20695000
C	-4.43579700	1.62956100	0.10345000	C	-4.43941300	1.67191500	0.17522600
H	3.85393700	-3.53139800	1.22080200	H	3.89631600	-3.46141600	1.29108800
H	-4.44117300	1.59757300	1.19485100	H	-4.42807800	1.59544900	1.26403500
H	4.65046500	-3.34757300	-0.34927200	H	4.75112500	-3.23596800	-0.24243400
H	-4.56610800	2.66882100	-0.20921700	H	-4.54280100	2.72654900	-0.09303600
H	3.53770600	-4.68057000	-0.07613500	H	3.68801600	-4.61856900	-0.02002500
H	-5.31412000	1.07710300	-0.24205200	H	-5.33960200	1.16036200	-0.17688800
H	-0.72641400	-1.24124600	0.00435000	H	-0.71677500	-1.25685300	-0.02679600
H	-0.14989300	-0.83319200	2.02795800	H	-0.14420600	-0.87955900	2.00140400
C	-1.00561400	-2.20722200	0.66037000	C	-0.98276800	-2.23104800	0.61937500
C	-2.44522800	-2.49255600	0.26490400	C	-2.42960400	-2.50940900	0.24756100
C	-2.79113200	-2.73802000	-1.06349000	C	-2.79945900	-2.74508000	-1.07611000
C	-4.10116100	-3.04038400	-1.40684600	C	-4.11749500	-3.03541100	-1.39877700
C	-5.08253400	-3.10636200	-0.42168700	C	-5.08252200	-3.09934400	-0.39761800
C	-3.42726700	-2.56886500	1.24613200	C	-3.39543600	-2.58404800	1.24499900
C	-4.74112800	-2.87231200	0.90418200	C	-4.71703500	-2.87578500	0.92366900
H	-2.02824300	-2.68585400	-1.83557100	H	-2.04988100	-2.69584700	-1.86117500
H	-4.35919400	-3.22840100	-2.44362300	H	-4.39416800	-3.21582100	-2.43204400
H	-6.10583100	-3.34739900	-0.68830500	H	-6.11198200	-3.33104100	-0.64822600
H	-3.12971000	-2.40336300	2.27525700	H	-3.07971500	-2.42736000	2.27005400
H	-5.49918800	-2.93542300	1.67794100	H	-5.46230400	-2.93799000	1.70978500
H	5.71974200	1.05747700	0.54277200	H	5.56764700	1.28746200	0.56243200
H	4.06192400	1.62836100	0.68490400	H	3.86914600	1.74294000	0.63866100
H	4.69641800	0.43627900	1.83213500	H	4.55285800	0.63450000	1.84306200
H	-0.96991400	5.36149300	0.90263700	H	-0.75891100	5.29062500	0.93096300
H	-1.20052100	4.07281100	2.07866700	H	-1.00827400	4.00274700	2.10409700
H	0.20100700	4.05163800	0.99258900	H	0.33677200	3.91285400	0.94958700
O	-0.77210700	-2.02566200	1.95488300	O	-0.72377500	-2.06842400	1.91262000
H	-0.37318200	-2.97287600	0.17285800	H	-0.35467900	-2.98445500	0.10733400
W	0.54494500	0.42982400	-0.24653400	W	0.55775000	0.45522900	-0.24243600
C	1.59922000	2.05091700	-0.36406500	C	0.32503600	0.09353700	-2.17069500
N	0.47547200	0.31505300	-2.05967800	N	1.50197100	1.93230400	-0.59948300
2W-cis + PhCOCH₃-TS				2W-trans + PhCOCH₃-TS			
O	2.02174900	2.92454100	-0.90284600	O	2.11800300	3.08115500	-0.33765000
P	-1.56915500	1.66097000	0.24068600	P	-1.57898300	1.65336500	0.22461700
P	2.63989400	-0.83930500	0.15311200	P	2.63076600	-0.85004400	0.12586200
C	-1.64663500	1.51780400	2.10088400	C	-1.65209400	1.49306400	2.08061700
C	2.59653700	-1.04289400	2.01342500	C	2.57214900	-1.06564800	1.98091600
H	-2.20378800	0.60082600	2.31419900	H	-2.19205700	0.56269000	2.27967800
H	2.09022800	-1.99015100	2.21930400	H	2.03880000	-2.00118600	2.16937900
H	-2.17694700	2.35298400	2.56344500	H	-2.20110500	2.31180800	2.54954500
H	3.59677600	-1.10841800	2.44794800	H	3.56690400	-1.16520600	2.42024000
C	-0.24774100	1.38473100	2.68272200	C	-0.25445400	1.37673500	2.67036900
C	1.81751200	0.09583900	2.65721900	C	1.81640300	0.08176500	2.63778400
H	-0.31630700	1.17769300	3.75907200	H	-0.32572500	1.17813100	3.74796400
H	1.67972700	-0.11221700	3.72665700	H	1.69269300	-0.12514300	3.70901800
H	0.32197100	2.30823500	2.55897200	H	0.30953600	2.30333700	2.54084100
H	2.37026800	1.03412200	2.57452800	H	2.37771000	1.01452500	2.54650900
N	0.50011200	0.29485800	2.01642900	N	0.49316600	0.28276300	2.01339300
C	2.93313800	-2.60745700	-0.41982900	C	2.85807900	-2.61303500	-0.48533800
C	-3.27316800	1.06334200	-0.26483200	C	-3.26142400	1.01760900	-0.30232100
H	2.04054800	-3.10392400	-0.03579100	H	1.91853000	-3.06971700	-0.17279000
H	-3.23184400	0.01070300	0.02521500	H	-3.19631900	-0.03776200	-0.02949600
C	4.27368000	0.02933700	-0.18861100	C	4.30347800	-0.05850500	-0.24051000

C	-1.60325200	3.50927000	-0.11349100	C	-1.68823000	3.49922300	-0.14860200
C	4.54142900	1.19712200	0.75888900	C	4.72411800	0.98774600	0.78921000
C	-0.71136300	4.31704200	0.82705400	C	-0.95085800	4.37658400	0.86033800
O	0.05952000	-0.25376400	-3.28378800	O	0.36038500	0.22992400	-3.25788300
H	-2.64222200	3.80654600	0.06680500	H	-2.75587300	3.73348700	-0.08085600
H	5.03939700	-0.73249100	-0.00730400	H	5.02248500	-0.88320100	-0.19489800
C	-1.25237600	3.81274200	-1.57079900	C	-1.21434400	3.80393000	-1.57002600
C	4.37116700	0.48695800	-1.64436500	C	4.33333100	0.53601800	-1.64897200
H	-1.85821000	3.24800500	-2.27806400	H	-1.71817900	3.19778800	-2.32252100
H	4.20318900	-0.32294400	-2.35344800	H	4.04639500	-0.18108300	-2.41767100
H	-0.20514500	3.59317500	-1.77568300	H	-0.14316200	3.63062700	-1.67129800
H	3.64987600	1.27529100	-1.85776300	H	3.66064300	1.38984600	-1.72810700
H	-1.41542300	4.87700100	-1.76811900	H	-1.40757600	4.85570300	-1.80312300
H	5.37167300	0.88927600	-1.83130400	H	5.34541600	0.88380000	-1.87784300
C	2.911111000	-2.75452400	-1.93975900	C	2.91455000	-2.69079000	-2.00987400
C	-3.49414000	1.11781300	-1.77467500	C	-3.45203600	1.09440300	-1.81549400
H	3.84114100	-2.40496400	-2.39271900	H	3.87685200	-2.34681300	-2.39565600
H	-3.67752800	2.13875500	-2.11793800	H	-3.62233600	2.12113700	-2.14905500
H	2.08389700	-2.20526200	-2.39130200	H	2.12581900	-2.09940200	-2.47876000
H	-2.64477600	0.71474000	-2.32822400	H	-2.59236100	0.69453200	-2.35659500
H	2.80287700	-3.81023300	-2.20564200	H	2.79367100	-3.72969800	-2.33089600
H	-4.37461300	0.52461300	-2.03441200	H	-4.32952400	0.50950100	-2.10300800
C	4.15564800	-3.28827300	0.19095300	C	4.00576400	-3.38574700	0.15940200
C	-4.42703500	1.72192500	0.48730200	C	-4.44410200	1.63305300	0.44084100
H	4.17475200	-3.22298300	1.28085700	H	3.95895000	-3.37686900	1.25043000
H	-4.32593400	1.63756800	1.57077500	H	-4.35580600	1.53426400	1.52442400
H	5.08920400	-2.86794800	-0.19081000	H	4.98201800	-2.99681400	-0.14043100
H	-4.53009500	2.78087200	0.23572000	H	-4.57445000	2.69269000	0.20506300
H	4.15422900	-4.35051300	-0.07197200	H	3.96926400	-4.43195100	-0.15981000
H	-5.36578200	1.23373700	0.20972100	H	-5.36465300	1.12295400	0.14231400
H	-0.47063100	-1.27191600	0.07385600	H	-0.46146200	-1.25685600	0.08524900
H	-0.06350300	-0.56967300	2.18200900	H	-0.07006000	-0.57956100	2.18094400
C	-1.22605200	-2.32115800	1.05752200	C	-1.24189400	-2.33496900	1.07152600
C	-2.55344100	-2.38574500	0.32870800	C	-2.55651000	-2.40093700	0.32291000
C	-2.65490800	-2.58366500	-1.04771700	C	-2.63396600	-2.57977000	-1.05776600
C	-3.89541900	-2.75457100	-1.64433900	C	-3.86278600	-2.75780500	-1.67553100
C	-5.05224700	-2.73853600	-0.87080900	C	-5.03159000	-2.76663200	-0.91960200
C	-3.71558700	-2.36958700	1.09759600	C	-3.73010900	-2.40851800	1.07414500
C	-4.95900200	-2.54471800	0.50129900	C	-4.96209000	-2.58990900	0.45607600
H	-1.75957400	-2.57075100	-1.65928700	H	-1.72814600	-2.53998100	-1.65286600
H	-3.96171300	-2.89516900	-2.71766700	H	-3.91148900	-2.88325800	-2.75170400
H	-6.02111700	-2.87681900	-1.33817200	H	-5.99143300	-2.90994400	-1.40378100
H	-3.62236100	-2.22477500	2.16771100	H	-3.65592800	-2.27662100	2.14746800
H	-5.85604800	-2.53541900	1.11125800	H	-5.86860900	-2.59868200	1.05185900
H	5.50823300	1.64488800	0.50981100	H	5.70882300	1.38168200	0.51999600
H	3.78785700	1.97904300	0.65713600	H	4.03495000	1.83275100	0.80878700
H	4.59207200	0.88570200	1.80408200	H	4.80697300	0.57813000	1.79777800
H	-0.79375800	5.37897000	0.57631000	H	-1.08843300	5.42843800	0.59160900
H	-0.99929800	4.21028500	1.87468500	H	-1.32407100	4.25316100	1.87879400
H	0.33846800	4.04073300	0.71791700	H	0.12235600	4.18209600	0.85416800
O	-1.19590500	-1.83612500	2.21836500	O	-1.22101000	-1.84176900	2.22677400
C	-0.35702100	-3.53791200	0.77307800	N	0.43240500	0.31194000	-2.07762900
H	-0.89748500	-4.41082600	1.15478500	C	1.51864900	2.07953200	-0.30681100
H	-0.16515600	-3.69467400	-0.28768100	C	-0.36861800	-3.54938900	0.79747700
H	0.57869200	-3.46062300	1.32375900	H	-0.90408200	-4.41807000	1.19628900
C	0.24389500	0.00760600	-2.16699100	H	-0.18993500	-3.72118600	-0.26308900
N	1.42682400	1.92566100	-0.62724200	H	0.57309300	-3.46430000	-1.33636500
W	0.52680100	0.40348900	-0.25582400	W	0.51726600	0.39277000	-0.26854700

Table S8. Computed Energetic Data For All Optimized Structures

H₂ HF= -1.178636 ZPE= 0.010066 NImag= 0 Htot = -1.165265 Gtot = -1.180063	Ph-C≡N HF=-324.462850 ZPE= 0.099090 NImag=0 Htot = -324.356685 Gtot = -324.394045
Ph-CH=NH HF= -325.672096 ZPE= 0.122298 NImag=0 Htot = -325.542367 Gtot = -325.580493	Ph-CH₂NH₂ HF= -326.893009 ZPE= 0.145861 NImag=0 Htot = -326.738985 Gtot = -326.778961
Ph-CH=NCH₂-Ph HF= -596.010269 ZPE= 0.230904 NImag=0 Htot = -595.765983 Gtot = -595.821242	Ph-CH₂NHCH₂-Ph HF= -597.227352 ZPE= 0.255195 NImag=0 Htot = -596.958369 Gtot = -597.014546
Ph-CH=N-Ph HF= -556.704384 ZPE= 0.202432 NImag=0 Htot = -556.489963 Gtot = -556.540191	Ph-CH₂NH-Ph HF= -557.923968 ZPE= 0.226160 NImag=0 Htot = -557.685119 Gtot = -557.737696
Ph-C≡CH HF= -308.368341 ZPE= 0.109270 NImag=0 Htot = -308.251652 Gtot = -308.289517	Ph-CH=CH₂ HF= -309.625103 ZPE= 0.132940 NImag=0 Htot = -309.484357 Gtot = -309.523956
Ph-CH₂CH₃ HF= -310.859083 ZPE= 0.156438 NImag=0 Htot = -310.694324 Gtot = -310.735616	Ph-CH=O HF=-345.550677 ZPE= 0.109586 NImag=0 Htot = -345.433783 Gtot = -345.471689
Ph-CH₂OH HF= -346.757584 ZPE= 0.132478 NImag=0 Htot = -346.617721 Gtot = -346.655623	Ph-CO-CH₃ HF= -384.871415 ZPE= 0.137519 NImag=0 Htot = -384.725019 Gtot = -384.766910
Ph-CH(OH)-CH₃ HF= -386.077179 ZPE= 0.161141 NImag=0	1Cr-cis-Cs HF= -1698.434145 ZPE= 0.517257 NImag=0

Htot = -385.906715 Gtot = -385.949373	Htot = -1697.883686 Gtot = -1697.979659
1Cr-trans-Cs HF= -1698.435891 ZPE= 0.517250 NImag=0 Htot = -1697.885437 Gtot = -1697.981546	1Cr-C1 HF= -1698.438722 ZPE= 0.517847 NImag= 0 Htot = -1697.888044 Gtot = -1697.982122
1Cr-C1-triplet HF= -1698.411827 ZPE= 0.51276 NImag=0 Htot = -1697.864167 Gtot = -1697.966886	2Cr-cis-Cs HF= -1699.63032673 ZPE= 0.538371 NImag=0 Htot = -1699.058738 Gtot = -1699.154320
2Cr-trans-Cs HF= -1699.634442 ZPE= 0.538207 NImag=0 Htot = -1699.063014 Gtot = -1699.158122	2Cr-C1 HF= -1699.62710259 ZPE= 0.538647 NImag=0 Htot = -1699.055342 Gtot = -1699.150012
1Mo-cis-Cs HF= -1679.71059594 ZPE= 0.516574 NImag=0 Htot = -1679.160580 Gtot = -1679.257603	1Mo-trans-Cs HF=-1679.711743 ZPE= 0.516295 NImag=0 Htot = -1679.161913 Gtot = -1679.259625
1Mo-C1 HF= -1679.71511108 ZPE= 0.516479 NImag=0 Htot = -1679.165308 Gtot = -1679.261198	1Mo-C1-triplet HF= -1679.662415 ZPE= 0.514632 NImag=0 Htot = -1679.113904 Gtot = -1679.212164
2Mo-cis-Cs HF= -1680.908875 ZPE= 0.536632 NImag=0 Htot = -1680.338459 Gtot = -1680.435621	2Mo-trans-Cs HF= -1680.908347 ZPE= 0.536611 NImag=0 Htot = -1680.337965 Gtot = -1680.434868
2Mo-C1 HF= -1680.905027 ZPE= 0.537308 NImag=0 Htot = -1680.334121 Gtot = -1680.430655	1W-cis-Cs HF= -1680.012956 ZPE= 0.516937 NImag=0 Htot = -1679.462683 Gtot = -1679.559296
1W-trans-Cs HF= -1680.014106 ZPE= 0.516715 NImag=0	1W-C1 HF= -1680.017393 ZPE= 0.516812 NImag=0

Htot = -1679.463978 Gtot = -1679.561342	Htot = -1679.467327 Gtot = -1679.563189
1W-C1-triplet HF= -1679.962700 ZPE= 0.515055 NImag=0 Htot = -1679.413885 Gtot = -1679.512088	2W-cis-Cs HF= -1681.21195076 ZPE= 0.537180 NImag=0 Htot = -1680.641116 Gtot = -1680.737998
2W-trans-Cs HF= -1681.210681 ZPE= 0.537014 NImag=0 Htot = -1680.639985 Gtot = -1680.736955	2W-C1 HF= -1681.20765166 ZPE= 0.537821 NImag=0 Htot = -1680.636328 Gtot = -1680.733042
1Cr-cis + H₂-TS HF= -1699.595777 ZPE= 0.532584 NImag= -898.8338 Htot = -1699.030124 Gtot = -1699.124827	1Cr-trans + H₂-TS HF= -1699.592918 ZPE= 0.532723 NImag= -680.5186 Htot = -1699.027111 Gtot = -1699.121754
2Cr-cis + PhCN-TS-H_M transfer HF= -2024.085209 ZPE= 0.638205 NImag= -266.6736 Htot = -2023.406946 Gtot = -2023.516881	2Cr-trans + PhCN-TS-H_M transfer HF= -2024.085942 ZPE= 0.638115 NImag= -351.3991 Htot = -2023.407816 Gtot = -2023.517739
2Cr-cis + PhCN-interm HF= -2024.089625 ZPE= 0.63916 NImag=0 Htot = -2023.410102 Gtot = -2023.520765	2Cr-trans + PhCN-interm HF= -2024.088369 ZPE= 0.639328 NImag=0 Htot = -2023.408768 Gtot = -2023.519194
2Cr-cis + PhCN-TS-H_N transfer HF=-2024.088810 ZPE= 0.636229 NImag= -760.4926 Htot = -2023.412493 Gtot = -2023.522712	2Cr-trans + PhCN-TS-H_N transfer HF=-2024.086583 ZPE= 0.636263 NImag= -944.9830 Htot = -2023.410295 Gtot = -2023.410295
2Cr-cis + PhCHNH-TS HF= -2025.284407 ZPE= 0.660985 NImag= -471.8223 Htot = -2024.583066 Gtot = -2024.693562	2Cr-trans + PhCHNH-TS HF= -2025.285579 ZPE= 0.660798 NImag= -509.3103 Htot = -2024.584418 Gtot = -2024.695098
2Cr-cis + PhCHNCH₂Ph-TS HF= -2295.605646 ZPE= 0.769612 NImag= -588.1071	2Cr-trans + PhCHNCH₂Ph-TS HF=-113,3043314 ZPE= 0.769705 NImag= -583.8970

Htot = -2294.789432 Gtot = -2294.916596	Htot = -2294.794414 Gtot = -2294.920163
2Cr-cis + PhCHNPh-TS HF= -2256.305976 ZPE= 0.741647 NImag= -542.5767 Htot = -2255.519164 Gtot = -2255.641352	2Cr-trans + PhCHNPh-TS HF= -2256.307231 ZPE= 0.741832 NImag= -637.7001 Htot = -2255.520307 Gtot = -2255.641835
2Cr-cis + PhCCH-TS HF= -2007.982791 ZPE= 0.647166 NImag= -489.2753 Htot = -2007.294598 Gtot = -2007.409226	2Cr-trans + PhCCH-TS HF=-2007.985371 ZPE= 0.647191 NImag=-547.2024 Htot = -2007.297194 Gtot = -2007.411223
2Cr-cis + PhCCH-TS-H_M transfer to Ph-<u>C</u> HF= -2007.973812 ZPE= 0.646810 NImag=-565.8722 Htot = -2007.286337 Gtot = -2007.397245	2Cr-trans + PhCCH-TS-H_M transfer to Ph-<u>C</u> HF= -2007.973928 ZPE= 0.646989 NImag=-675.2528 Htot = -2007.286395 Gtot = -2007.397514
2Cr-cis + PhCCH-interm HF=-2007.978392 ZPE= 0.650442 NImag=0 Htot = -2007.287133 Gtot = -2007.398869	2Cr-trans + PhCCH-interm HF= -2007.976905 ZPE= 0.650438 NImag=0 Htot = -2007.285706 Gtot = -2007.397638
2Cr-cis + PhCCH-TS-H_N transfer to <u>C</u>-H HF=-2007.975161 ZPE= 0.648481 NImag= -565.9038 Htot = -2007.286242 Gtot = -2007.396668	2Cr-trans + PhCCH-TS-H_N transfer to <u>C</u>-H HF= -2007.973673 ZPE= 0.648188 NImag= -560.3261 Htot = -2007.285062 Gtot = -2007.395654
2Cr-cis + PhCHCH₂-TS-H_M transfer HF= -2009.235073 ZPE= 0.671233 NImag= -587.5247 Htot = -2008.522812 Gtot = -2008.636422	2Cr-trans + PhCHCH₂-TS-H_M transfer HF= -2009.237577 ZPE= 3,18554 NImag= -637.7881 Htot = -2008.52517 Gtot = -2008.637397
2Cr-cis + PhCHCH₂-interm HF= -2009.241347 ZPE= 0.67379 NImag=0 Htot = -2008.526329 Gtot = -2008.639162	2Cr-trans + PhCHCH₂-interm HF= -2009.240849 ZPE= 0.673863 NImag=0 Htot = -2008.525852 Gtot = -2008.638096
2Cr-cis + PhCHCH₂-TS-H_N transfer HF= -2009.24043 ZPE= 0.670783 NImag= -612.2189	2Cr-trans + PhCHCH₂-TS-H_N transfer HF= -2009.238386 ZPE= 0.670461 NImag= -876.7163

Htot = -2008.528788 Gtot = -2008.641016	Htot = -2008.52705 Gtot = -2008.639056
2Cr-cis + PhCHO-TS-H_M transfer HF= -2045.177037 ZPE= 0.649012 NImag= -228.6489 Htot = -2044.487679 Gtot = -2044.599331	2Cr-trans + PhCHO-TS-H_M transfer HF= -2045.179995 ZPE= 0.649194 NImag= -319.0508 Htot = -2044.490525 Gtot = -2044.601149
2Cr-cis + PhCHO-interm HF= -2045.18804 ZPE= 0.650691 NImag= 0 Htot = -2044.496767 Gtot = -2044.608543	2Cr-trans + PhCHO-interm HF= -2045.187458 ZPE= 0.650492 NImag=0 Htot = -2044.496337 Gtot = -2044.607917
2Cr-cis + PhCHO-TS-H_N transfer HF= -2045.188631 ZPE= 0.64917 NImag= -48.8347 Htot = -2044.499409 Gtot = -2044.609702	2Cr-trans + PhCHO-TS-H_N transfer HF=-2045.187237 ZPE= 0.647875 NImag=-429.6125 Htot = -2044.498944 Gtot = -2044.610746
2Cr-cis + PhCOCH₃-TS HF= -2084.482635 ZPE= 0.67706 NImag=-448.0065 Htot = -2083.764056 Gtot = -2083.876428	2Cr-trans + PhCOCH₃-TS HF= -2084.484868 ZPE= 0.677214 NImag=-521.3906 Htot = -2083.766124 Gtot = -2083.879005
1Mo-cis + H₂-TS HF= -1680.872893 ZPE= 0.531036 NImag= -944.5296 Htot = -1680.308259 Gtot = -1680.404911	1Mo-trans + H₂-TS HF= -1680.868998 ZPE= 0.530731 NImag= -804.2043 Htot = -1680.30452 Gtot = -1680.40132
2Mo-cis + PhCN-TS-H_M transfer HF= -2005.365167 ZPE= 0.636259 NImag= -250.8588 Htot = -2004.688101 Gtot = -2004.80138	2Mo-trans + PhCN-TS-H_M transfer HF= -2005.362539 ZPE= 0.636146 NImag=-308.8044 Htot = -2004.685578 Gtot = -2004.798739
2Mo-cis + PhCN-interm HF= -2005.368252 ZPE= 0.637523 NImag=0 Htot = -2004.689728 Gtot = -2004.803232	2Mo-trans + PhCN-interm HF= -2005.3644 ZPE= 0.637356 NImag=0 Htot = -2004.686009 Gtot = -2004.799444
2Mo-cis + PhCN-TS-H_N transfer HF= -2005.367106 ZPE= 0.63471 NImag= -832.4556	2Mo-trans + PhCN-TS-H_N transfer HF= -2005.362736 ZPE= 0.634523 NImag= -907.7142

Htot = -2004.691732 Gtot = -2004.804412	Htot = -2004.687517 Gtot = -2004.800184
2Mo-cis + PhCHNH-TS HF= -2006.56487 ZPE= 0.659455 NImag= -441.943 Htot = -2005.864495 Gtot = -2005.977334	2Mo-trans + PhCHNH-TS HF= -2006.562726 ZPE= 0.659171 NImag= -468.5723 Htot = -2005.862535 Gtot = -2005.975746
2Mo-cis + PhCHNCH₂Ph-TS HF= -2276.890797 ZPE= 0.768219 NImag= -466.3936 Htot = -2276.075521 Gtot = -2276.203236	2Mo-trans + PhCHNCH₂Ph -TS HF= -2276.888774 ZPE= 0.76806 NImag= -520.8288 Htot = -2276.073547 Gtot = -2276.202495
2Mo-cis + PhCHNPh-TS HF= -2237.587423 ZPE= 0.740058 NImag= -498.2876 Htot = -2236.801581 Gtot = -2236.926254	2Mo-trans + PhCHNPh-TS HF= -2237.585742 ZPE= 0.739942 NImag= -573.9478 Htot = -2236.799933 Gtot = -2236.924746
2Mo-cis + PhCCH-TS HF= -1989.260784 ZPE= 0.64546 NImag= -508.465 Htot = -1988.573654 Gtot = -1988.690865	2Mo-trans + PhCCH-TS HF= -1989.258983 ZPE= 0.645545 NImag= -546.8679 Htot = -1988.571808 Gtot = -1988.688153
2Mo-cis + PhCCH-TS-H_M transfer to Ph-C HF=-1989.252808 ZPE= 0.645122 NImag= -548.7414 Htot = -1988.566329 Gtot = -1988.680342	2Mo-trans + PhCCH-TS-H_M transfer to Ph-C HF= -1989.249621 ZPE= 0.644905 NImag= -632.162 Htot = -1988.563309 Gtot = -1988.677895
2Mo-cis + PhCCH-interm HF= -1989.256772 ZPE= 0.649078 NImag= 0 Htot = -1988.566336 Gtot = -1988.680402	2Mo-trans + PhCCH-interm HF= -1989.252299 ZPE= 0.648709 NImag= 0 Htot = -1988.562128 Gtot = -1988.677014
2Mo-cis + PhCCH-TS-H_N transfer to C-H HF= -1989.253133 ZPE= 0.646758 NImag= -562.8082 Htot = -1988.565276 Gtot = -1988.678542	2Mo-trans + PhCCH-TS-H_N transfer to C-H HF= -1989.248588 ZPE= 0.646177 NImag= -559.3783 Htot = -1988.561221 Gtot = -1988.674807
2Mo-cis + PhCHCH₂-TS-H_M transfer HF= -1990.514063 ZPE= 0.669776 NImag= -599.4169	2Mo-trans + PhCHCH₂-TS-H_M transfer HF= -1990.512265 ZPE= 0.669439 NImag= -632.6759

Htot = -1989.802768 Gtot = -1989.917973	Htot = -1989.801146 Gtot = -1989.916785
2Mo-cis + PhCHCH₂-interm HF= -1990.519189 ZPE= 0.672158 NImag=0 Htot = -1989.80525 Gtot = -1989.92006	2Mo-trans + PhCHCH₂-interm HF= -1990.515335 ZPE= 0.67169 NImag=0 Htot = -1989.80172 Gtot = -1989.916986
2Mo-cis + PhCHCH₂-TS-H_N transfer HF= -1990.518356 ZPE= 0.669278 NImag=-578.5316 Htot = -1989.807653 Gtot = -1989.922189	2Mo-trans + PhCHCH₂-TS-H_N transfer HF=-1990.513865 ZPE= 0.668911 NImag=-703.5043 Htot = -1989.803481 Gtot = -1989.917601
2Mo-cis + CN-Ph-CHCH₂-TS-H_M transfer (CN bond) HF= -2082.758163 ZPE= 0.66893 NImag= -252.8325 Htot = -2082.045918 Gtot = -2082.165181	2Mo-cis + CN-Ph-CHCH₂-TS- H_M transfer (C=C bond) HF= ZPE= 0.668626 NImag= -491.2152 Htot = -2082.037592 Gtot = -2082.157453
2Mo-cis + CN-Ph-CHCH₂-interm (CN bond) HF= -2082.761279 ZPE= 0.670437 NImag= 0 Htot = -2082.047401 Gtot = -2082.166774	2Mo-cis + CN-Ph-CHCH₂-interm (C=C bond) HF= -2082.760318 ZPE= 0.671789 NImag= 0 Htot = -2082.044833 Gtot = -2082.164603
2Mo-cis + CN-Ph-CHCH₂-TS-H_N transfer (CN bond) HF= -2082.760055 ZPE= 0.667183 NImag= -830.7889 Htot = -2082.049625 Gtot = -2082.169166	2Mo-cis + CN-Ph-CHCH₂-TS- H_M transfer (C=C bond) HF= -2082.757247 ZPE= 0.668167 NImag= -1014.8742 Htot = -2082.045763 Gtot = -2082.164572
Fe + CN-Ph-CHCH₂-TS-H_M transfer (CN bond) HF= -2009.26734 ZPE= 0.669955 NImag= -271.355 Htot = -2008.556815 Gtot = -2008.669635	Fe + CN-Ph-CHCH₂-TS- H_M transfer (C=C bond) HF= -2009.26286 ZPE= 0.669701 NImag= -445.7233 Htot = -2008.552496 Gtot = -2008.666156
Fe + CN-Ph-CHCH₂-interm (CN bond) HF= -2009.269869 ZPE= 0.671404 NImag=0 Htot = -2008.557755 Gtot = -2008.670263	Fe + CN-Ph-CHCH₂-interm (C=C bond) HF= -2009.272126 ZPE= 0.672639 NImag= 0 Htot = -2008.558427 Gtot = -2008.672326
Fe + CN-Ph-CHCH₂-TS-H_N transfer (CN bond) HF= -2009.268145 ZPE= 0.667969 NImag= -952.8209	Fe + CN-Ph-CHCH₂-TS-H_N transfer (C=C bond) HF= -2009.267906 ZPE= 0.668787 NImag= -1120.7845

Htot = -2008.559532 Gtot = -2008.672485	Htot = -2008.558339 Gtot = -2008.671396
2Mo-cis + PhCHO-TS-H_M transfer HF= -2026.458394 ZPE= 0.647515 NImag= -211.4837 Htot = -2025.770003 Gtot = -2025.883717	2Mo-trans + PhCHO-TS-H_M transfer HF=-2026.457358 ZPE= 0.647461 NImag= -282.1492 Htot = -2025.768978 Gtot = -2025.882145
2Mo-cis + PhCHO-interm HF= -2026.46714 ZPE= 0.648752 NImag= 0 Htot = -2025.77725 Gtot = -2025.891389	2Mo-trans + PhCHO-interm HF= -2026.465003 ZPE= 0.648797 NImag= 0 Htot = -2025.774962 Gtot = -2025.889196
2Mo-cis + PhCHO-TS-H_N transfer HF= -2026.468611 ZPE= 0.647011 NImag= -207.6561 Htot = -2025.780836 Gtot = -2025.89453	2Mo-trans + PhCHO-TS-H_N transfer HF= -2026.464783 ZPE= 0.646358 NImag= -437.5335 Htot = -2025.777486 Gtot = -2025.89114
2Mo-cis + PhCOCH₃-TS HF= -2065.766098 ZPE= 0.675714 NImag=-380.6443 Htot = -2065.048296 Gtot = -2065.162971	2Mo-trans + PhCOCH₃-TS HF= -2065.765142 ZPE= 0.67552 NImag= -430.5312 Htot = -2065.047403 Gtot = -2065.162753
1W-cis + H₂-TS HF= -1681.173302 ZPE= 0.531426 NImag= -952.0228 Htot = -1680.608371 Gtot = -1680.704822	1W-trans + H₂-TS HF= -1681.169136 ZPE= 0.531211 NImag=-821.2732 Htot = -1680.604325 Gtot = -1680.700644
2W-cis + PhCN-TS-H_M transfer HF= -2005.666868 ZPE= 0.636618 NImag= -215.147 Htot = -2004.989671 Gtot = -2005.102118	2W-trans + PhCN-TS-H_M transfer HF= -2005.663499 ZPE= 0.636534 NImag=0 Htot = -2004.986438 Gtot = -2005.098606
2W-cis + PhCN-interm HF= -2005.667451 ZPE= 0.637401 NImag=0 Htot = -2004.989116 Gtot = -2005.102312	2W-trans + PhCN-interm HF= -2005.663582 ZPE= 0.637125 NImag=0 Htot = -2004.985447 Gtot = -2005.098734
2W-cis + PhCN-TS-H_N transfer HF= -2005.666069 ZPE= 0.634862 NImag= -820.9509	2W-trans + PhCN-TS-H_N transfer HF=-113,3043314 ZPE= 0.634781 NImag= -874.9568

Htot = -2004.990687 Gtot = -2005.102921	Htot = -2004.986421 Gtot = -2005.098409
2W-cis + PhCHNH-TS HF= -2006.865642 ZPE= 0.659533 NImag= -344.4175 Htot = -2006.165349 Gtot = -2006.27767	2W-trans + PhCHNH-TS HF= -2006.862896 ZPE= 0.659107 NImag= -264.8691 Htot = -2006.162991 Gtot = -2006.275519
2W-cis + PhCHNCH₂Ph-TS HF= -2277.19157 ZPE= 0.768514 NImag= -397.5103 Htot = -2276.376157 Gtot = -2276.503457	2W-trans + PhCHNCH₂Ph -TS HF= -2277.189108 ZPE= 0.7684 NImag= -391.6849 Htot = -2276.373772 Gtot = -2276.501689
2W-cis + PhCHNPh-TS HF= -2237.888631 ZPE= 0.740429 NImag= -505.8788 Htot = -2237.102544 Gtot = -2237.226731	2W-trans + PhCHNPh -TS HF= -2237.886435 ZPE= 0.740496 NImag= -568.3778 Htot = -2237.100303- Gtot = -2237.2247
2W-cis + PhCCH-TS HF= -1989.561415 ZPE= 0.645822 NImag= -499.3745 Htot = -1988.874095 Gtot = -1988.99045	2W-trans + PhCCH-TS HF= -1989.558984 ZPE= 0.645852 NImag= -512.6384 Htot = -1988.871647 Gtot = -1988.987693
2W-cis + PhCCH-TS-H_M transfer to Ph-<u>C</u> HF= -1989.55484 ZPE= 0.645571 NImag= -553.2234 Htot = -1988.868116 Gtot = -1988.981512	2W-trans + PhCCH-TS-H_M transfer to Ph-<u>C</u> HF= -1989.551223 ZPE= 0.645341 NImag= -626.466 Htot = -1988.86469 Gtot = -1988.978442
2W-cis + PhCCH-interm HF= -1989.553864 ZPE= 0.648753 NImag=0 Htot = -1988.863857 Gtot = -1988.977492	2W-trans + PhCCH-interm HF= -1989.549434 ZPE= 0.648546 NImag=0 Htot = -1988.859594 Gtot = -1988.973629
2W-cis + PhCCH-TS-H_N transfer to <u>C</u>-H HF= -1989.552276 ZPE= 0.646035 NImag= -460.5729 Htot = -1988.865049 Gtot = -1988.978321	2W-trans + PhCCH-TS-H_N transfer to <u>C</u>-H HF= -1989.54815 ZPE= 0.645984 NImag= -528.9298 Htot = -1988.860986 Gtot = -1988.974505
2W-cis + PhCHCH₂-TS-H_M transfer HF= -1990.81422 ZPE= 0.670151 NImag= -557.2345	2W-trans + PhCHCH₂-TS-H_M transfer HF= -1990.811793 ZPE= 0.669879 NImag= -529.3969

Htot = -1990.102705 Gtot = -1990.217384	Htot = -1990.100449 Gtot = -1990.215052
2W-cis + PhCHCH₂-interm HF= -1990.816205 ZPE= 0.67203 NImag=0 Htot = -1990.102521 Gtot = -1990.21739	2W-trans + PhCHCH₂-interm HF= -1990.812625 ZPE= 0.671658 NImag=0 Htot = -1990.099249 Gtot = -1990.213943
2W-cis + PhCHCH₂-TS-H_N transfer HF= -1990.815708 ZPE= 0.669743 NImag= -418.6072 Htot = -1990.104751 Gtot = -1990.218745	2W-trans + PhCHCH₂-TS-H_N transfer HF= -1990.811569 ZPE= 0.669351 NImag= -547.5947 Htot = -1990.100959 Gtot = -1990.214522
2W-cis + PhCHO-TS-H_M transfer HF= -2026.760024 ZPE= 0.647984 NImag= -240.9945 Htot = -2026.071329 Gtot = -2026.184502	2W-trans + PhCHO-TS-H_M transfer HF= -2026.758472 ZPE= 0.64787 NImag= -283.1497 Htot = -2026.069834 Gtot = -2026.182641
2W-cis + PhCHO-interm HF= -2026.766121 ZPE= 0.648493 NImag=0 Htot = -2026.076503 Gtot = -2026.19077	2W-trans + PhCHO-interm HF= -2026.762828 ZPE= 0.648716 NImag=0 Htot = -2026.07296 Gtot = -2026.187112
2W-cis + PhCHO-TS-H_N transfer HF= -2026.766187 ZPE= 0.647693 NImag= -77.1697 Htot = -2026.078047 Gtot = -2026.190229	2W-trans + PhCHO-TS-H_N transfer HF= -2026.762734 ZPE= 0.646879 NImag= -263.5586 Htot = -2026.075169 Gtot = -2026.188023
2W-cis + PhCOCH₃-TS HF= -2066.067295 ZPE= 0.67612 NImag= -380.7314 Htot = -2065.349238 Gtot = -2065.463565	2W-trans + PhCOCH₃-TS HF= -2066.066082 ZPE= 0.676005 NImag= -416.5481 Htot = -2065.348063 Gtot = -2065.462916