What is the Preferred Structure of the Meisenheimer-Wheland Complex between sym-Triaminobenzene and 4, 6-Dinitrobenzofuroxan?

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1. Full citation of Ref. 16

2. Optimized Cartesian coordinates of the *N*-piperidyl substituted M-W complexes at the M06-2X/6-311+G* level of theory, as well as the figures showing the benzene-benzene ring separation and displacement

1. Full citation of Ref. 16

Ref.14. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E. ; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

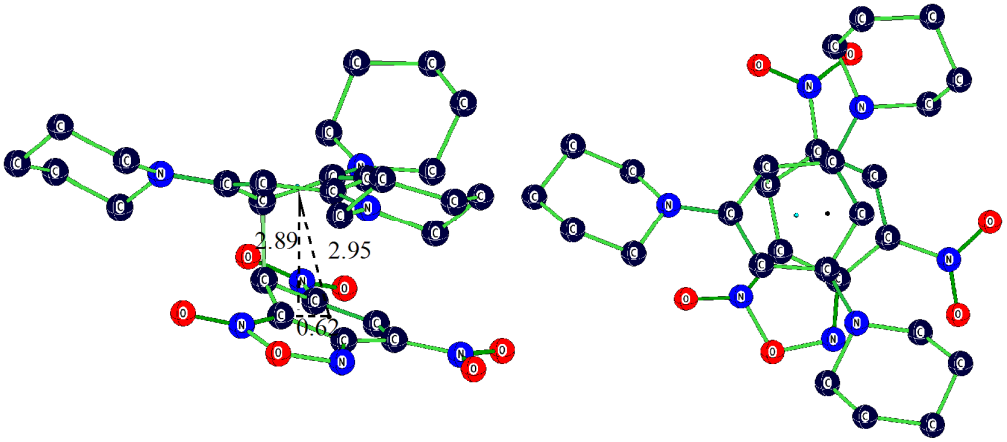
2. Optimized Cartesian coordinates of the *N*-piperidyl substituted M-W complexes at the M06-2X/6-311+G* level of theory, as well as the figures showing the benzene-benzene ring separation and displacement

s-syn

C	-1.78996200	-0.64441600	0.58082900
C	0.51859500	-1.25038400	1.06465300
C	-0.03345700	1.10838300	0.91880000
C	-0.86574400	-1.59770400	0.94311300
C	-1.27621100	0.70084200	0.16488100
C	0.86705500	0.13072400	1.23676600
H	-1.16525600	-2.62947900	0.97935600
H	-2.04036900	1.46236500	0.25406400
H	1.81320300	0.38157400	1.68986800
N	0.22382700	2.43282300	1.02420000
C	1.58836000	2.93420600	1.19227600
C	1.85863300	3.32430400	2.64374600
C	0.83180100	4.36852000	3.08907000
C	-0.59373000	3.88227600	2.82208500
C	-0.77607000	3.45391200	1.36296300
H	2.29506000	2.20059800	0.80452900
H	1.66763400	3.81931800	0.54870200
H	2.87485500	3.71537900	2.73676700
H	1.78941600	2.43399200	3.27948500
H	0.96010500	4.60657300	4.14776600
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H	-1.31719200	4.66912200	3.05280000
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H	-0.63356500	4.30477100	0.68800100
N	-3.12698100	-0.88340600	0.50202000
C	-3.95553400	-0.18850300	-0.49958600
C	-5.42619400	-0.16528100	-0.10566700
C	-5.94035900	-1.58123200	0.12434600
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H	-5.87672900	-2.14971600	-0.81080000
H	-5.38229200	-3.28670800	1.34997600
H	-5.22090100	-1.72602600	2.14714000
H	-3.03245600	-2.58472700	1.69063000
H	-3.39158000	-2.89297100	-0.01957300
N	1.48445700	-2.17692200	1.06413500
C	1.25189500	-3.62456900	1.03565000
C	2.09705600	-4.31480900	2.10737600
C	3.58052000	-3.98598100	1.95310400
C	3.78635400	-2.47220100	1.90981200
C	2.90428300	-1.86130000	0.82814900
H	0.20273500	-3.84648700	1.19691200
H	1.52084800	-3.98370700	0.03489300
H	1.92917000	-5.39295500	2.04232900
H	1.74393700	-3.99024600	3.09235600
H	4.15557200	-4.43392700	2.76686700
H	3.95413000	-4.42203900	1.01955700
H	4.82852700	-2.22773900	1.69156900
H	3.53924800	-2.02812900	2.88078900
H	3.04363900	-0.78859600	0.73911900
H	3.15917000	-2.27836300	-0.15330100
C	-0.89729400	0.68444300	-1.42356100
C	1.25747800	-0.67733300	-1.98556500
C	2.03424100	0.53086600	-1.93802200
C	1.34945200	1.74502100	-1.92310200
C	-0.01681300	1.84118500	-1.79597900
H	-1.85355800	0.72753900	-1.94706400
H	1.92728100	2.65871100	-2.00525500
N	-0.61475000	3.11911900	-1.70774300

O	0.06669100	4.13087500	-1.81926200
O	-1.82884200	3.15634900	-1.47720400
N	3.44651900	0.50437100	-1.90609400
O	4.05756900	1.56468400	-1.81483500
O	3.99285100	-0.59324600	-1.93324600
C	-0.15624400	-0.53916700	-1.82371200
N	1.56977500	-1.93074900	-2.20474200
N	-0.66722400	-1.73374900	-1.99849100
O	-1.81415800	-2.17728800	-1.96458000
O	0.37350900	-2.62015000	-2.21548200

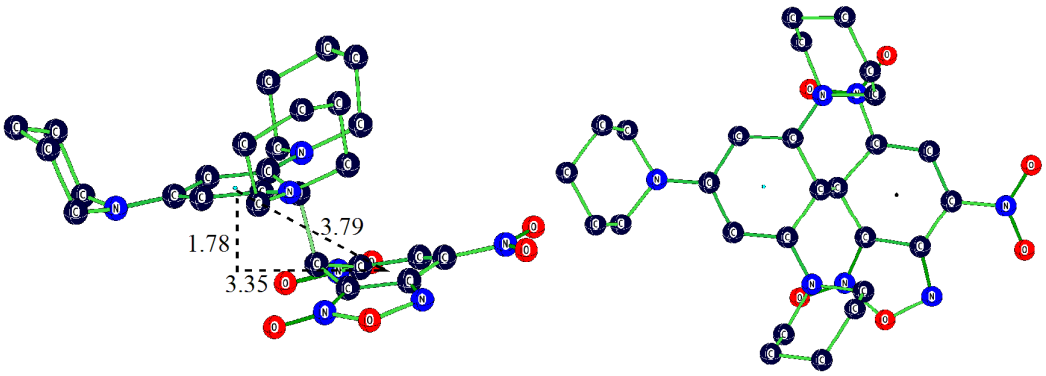


s-anti

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C	0.13216800	0.07369000	0.15963800
C	-1.82185900	-1.38505800	-0.20953700
H	-2.76328600	1.90423000	-0.26203500
H	0.92906800	0.17102100	0.88560100
H	-2.28660400	-2.35344900	-0.23962800
N	0.22352300	-2.32425800	0.63334900
C	-0.24677100	-3.70120300	0.47390000
C	-0.79717300	-4.22288200	1.80043000
C	0.29525900	-4.14907500	2.87159300
C	0.90676700	-2.74784200	2.94655200
C	1.35915200	-2.27051400	1.56393000
H	-0.95029100	-3.75693300	-0.35200300

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H	-1.65943800	-3.61368000	2.09623700
H	-0.10082600	-4.44294200	3.84650600
H	1.08463100	-4.86799000	2.62227200
H	1.76277400	-2.73803400	3.62615900
H	0.16949700	-2.03750400	3.33862200
H	1.79306400	-1.27578800	1.61563800
H	2.14115400	-2.92725800	1.16872900
N	-0.30116600	2.44429000	0.56674800
C	0.83034800	2.68690600	1.47020000
C	0.31270000	3.25750600	2.79410800
C	-0.52105400	4.52037600	2.56857700
C	-1.62387700	4.27372300	1.53628700
C	-1.00760000	3.69257800	0.26612300
H	1.40591000	1.78142500	1.63929900
H	1.49817000	3.40108000	0.97562900
H	1.16468500	3.47079500	3.44504500
H	-0.29464500	2.49269700	3.29195800
H	-0.94555300	4.86815400	3.51342900
H	0.13425400	5.31925700	2.20244700
H	-2.14626600	5.20437000	1.30046300
H	-2.36562500	3.57176800	1.93532100
H	-1.72316100	3.52532000	-0.53362400
H	-0.25552100	4.38013000	-0.13852800
N	-3.79456600	-0.36997000	-1.14872400
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C	-5.66585300	0.78212000	-0.08021500
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C	-4.51571100	-1.64324100	-1.19559600
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H	-5.98518100	-2.68830200	0.00085600
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H	-3.82823900	-2.47872200	-1.28124300
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C	0.87957000	0.16593500	-1.29014500
C	3.16277000	-0.95635400	-0.86856700
C	3.66703700	0.31670600	-0.42144800

C	2.97110200	1.46248600	-0.80180200
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H	0.11126900	0.12551300	-2.06274800
H	3.46138300	2.42179100	-0.68186000
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O	1.66027600	3.68036900	-1.64664700
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N	4.94476500	0.43288000	0.19540700
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O	5.56250300	-0.59871200	0.40370700
C	1.83482800	-0.96231100	-1.39183800
N	3.69372200	-2.14991100	-0.95555400
N	1.59527800	-2.18447200	-1.80320400
O	0.61984500	-2.74094800	-2.29582700
O	2.72959500	-2.94516800	-1.54382200



p-p

C	1.91553200	-0.11895200	0.50708000
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C	1.36482700	1.17085800	0.57552400
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C	-0.81911800	0.22404400	1.00138200
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H	1.48116700	-2.22006700	0.51483900
H	-1.87878100	0.36171800	1.14320900
N	-1.17012000	-2.16976800	0.92915500
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C	-1.97339100	-2.42434000	3.24422700

C	-1.29300500	-3.79421200	3.33931000
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C	-0.61076000	-3.52168900	0.94471300
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H	-2.86396800	-2.39425800	3.87844600
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H	-1.41431000	-4.19547700	0.62800100
N	3.30420800	-0.27304600	0.38809000
C	3.85737300	-1.61863600	0.47976900
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C	5.49580100	0.66413600	-0.26246100
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H	3.34351400	-2.15398700	1.27902700
H	3.69139700	-2.17303500	-0.46094100
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H	5.47276000	-1.16684000	1.81215400
H	7.17824100	-0.66692200	0.08582800
H	6.07807900	-1.19055400	-1.18542000
H	5.98668500	1.27587400	-1.02432700
H	5.61251600	1.17466000	0.69951500
H	3.56118300	1.53947800	-0.64420700
H	3.90511700	0.10253400	-1.59592900
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C	0.21254900	3.78164100	0.40330600
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C	-0.25449900	4.72267600	2.67765400
C	-1.16018600	3.51548700	2.93052000
C	-1.70060300	2.96961500	1.60665900
H	0.96115000	3.52516200	-0.34854100
H	-0.45399000	4.52163300	-0.05561500
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H	1.53292800	3.65150400	2.10663800
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H	-0.86128800	5.54688600	2.28209900
H	-1.99276100	3.78866300	3.58521800
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H	-2.30365700	3.73298100	1.10273500
C	-0.63148300	1.29631500	-2.17743800
C	-2.60996600	-0.10547500	-1.51278600
C	-1.84071400	-1.28549400	-1.80049100
C	-0.55311700	-1.16024500	-2.20709600
C	0.03261400	0.12964400	-2.38342000
H	-0.16936500	2.26846600	-2.28945400
H	0.04334200	-2.04491900	-2.38825800
N	1.45291300	0.19345800	-2.75589900
O	2.04535600	-0.85755000	-2.87343900
O	1.94197400	1.29088100	-2.91285500
N	-2.39799800	-2.61764900	-1.59074800
O	-1.71435600	-3.57106700	-1.90191600
O	-3.51480900	-2.67469300	-1.12579000
C	-1.96387300	1.14148100	-1.75477500
N	-3.81377100	0.07707200	-1.02776800
N	-2.83713300	2.08764700	-1.39328200
O	-2.81105500	3.29675900	-1.39460800
O	-3.96784700	1.43849900	-0.94631600

