

Electronic supplementary information for:

Theoretical studies on the spin trapping of 2-chloro-5-hydroxy-1,4-benzoquinone radical by 5,5-dimethyl-1-pyrroline *N*-oxide (DMPO): The identification of the C-O bonding spin adduct

Wenling Feng^a, Cong Ren^a, Weihua Wang^{*,a}, Chao Guo^a, Qiao Sun^b, Ping Li^{*,a}

^a Key Laboratory of Life-Organic Analysis, School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu, 273165, P. R. China

^b Collaborative Innovation Center of Radiation Medicine of Jiangsu Higher Education Institutions, School for Radiological and Interdisciplinary Sciences, Soochow University, Suzhou, 215123, P. R. China

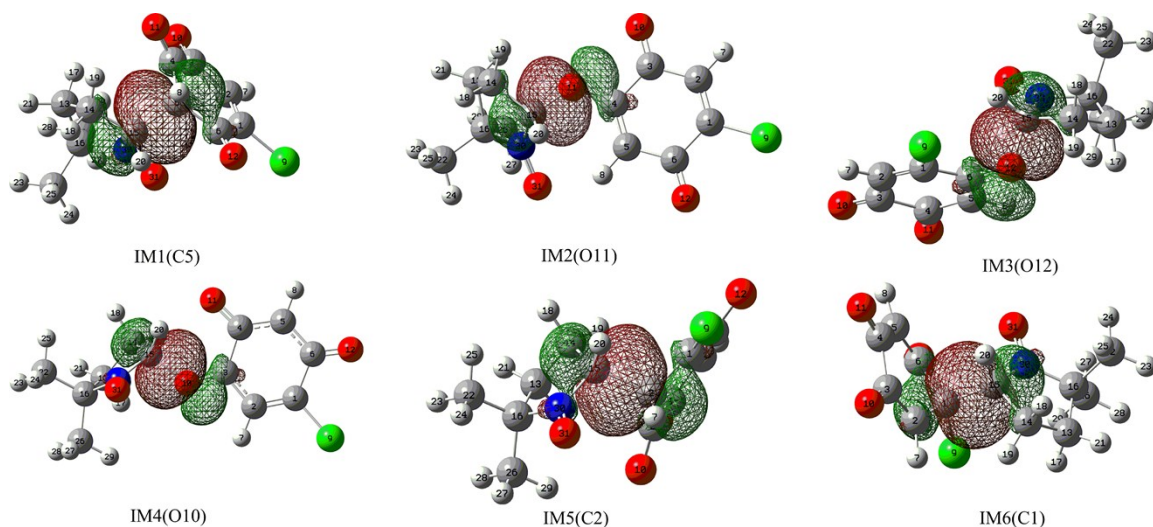


Fig. S1 Schematic graphs of the NBO orbital associated with the interaction between DMPO and CBQ radical on the basis of the alpha orbitals. The isodensity contours are 0.004 electron/bohr³.

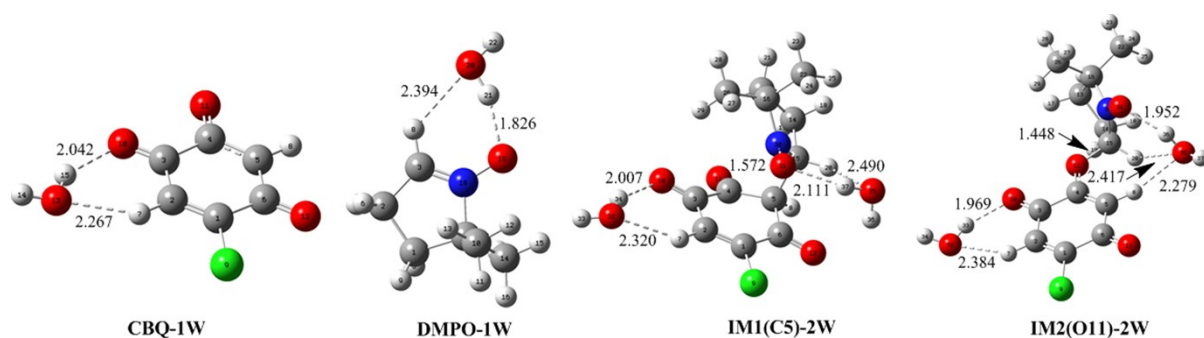


Fig. S2 The optimized complexes of water molecule with CBQ, DMPO, IM1(C5), and IM2(O11) at the B3LYP/6-311++G(d,p) level of theory.

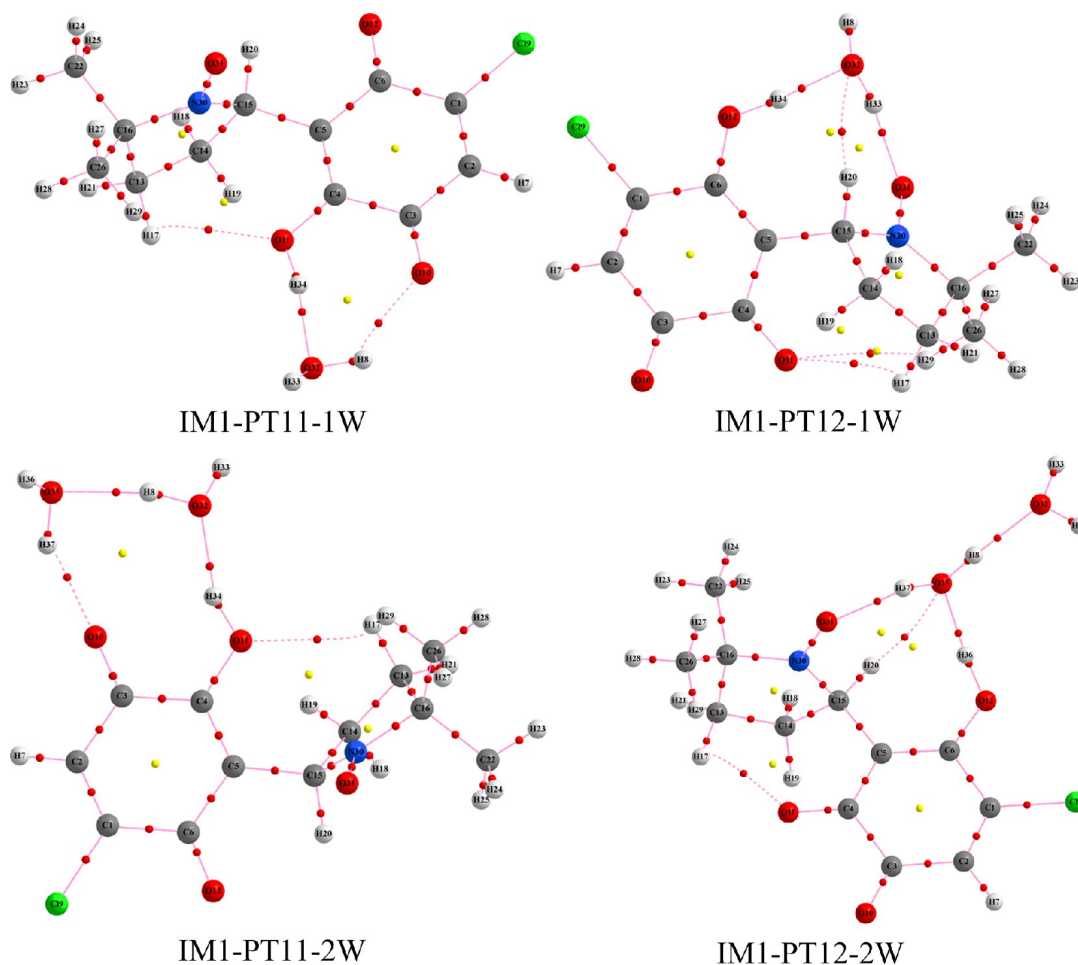


Fig. S3 Molecular graphs of the water-assisted keto-enol tautomerization products, where the BCP and RCP are denoted as small red and yellow dots, respectively.

Table S1 Topological analyses for the keto-enol tautomerization products of the three most stable spin adducts ^a

Complexes	BCP	ρ_{bcp}	$\nabla^2\rho_{\text{bcp}}$	V_{bcp}	G_{bcp}	H_{bcp}
IM1-PT11	C5 - C15	0.2406	-0.5345	-0.2448	0.0556	-0.1892
	H8 - O31	0.0506	0.1457	-0.0501	0.0433	-0.0068
IM1-PT12	O11 - H17	0.0090	0.0313	-0.0058	0.0068	0.0010
	O11 - H19	0.0155	0.0572	-0.0104	0.0124	0.0019
	C5 - C15	0.2401	-0.5287	-0.2449	0.0564	-0.1885
	H8 - O31	0.0571	0.1409	-0.0566	0.0459	-0.0107
IM2-PT11	O11 - C15	0.1993	-0.2918	-0.3266	0.1268	-0.1998
	O10 - H19	0.0146	0.0476	-0.0088	0.0103	0.0015
IM2-PT12	O11 - C15	0.2334	-0.4075	-0.4660	0.1821	-0.2839
IM3-PT11	O12 - C15	0.2276	-0.4083	-0.4281	0.1630	-0.2651
	C19 - H20	0.0123	0.0436	-0.0070	0.0089	0.0020
	C5 - H29	0.0014	0.0044	-0.0005	0.0008	0.0003
IM3-PT12	O12 - C15	0.1821	-0.1951	-0.2640	0.1076	-0.1564
	C19 - H20	0.0080	0.0276	-0.0041	0.0055	0.0014
	C5 - H29	0.0049	0.0113	-0.0020	0.0024	0.0004

^a The ρ_{bcp} , $\nabla^2\rho_{\text{bcp}}$, V_{bcp} , G_{bcp} , and H_{bcp} is electron density, the Laplacian of the electron density, potential energy density, kinetic energy density, and energy density at the BCP, respectively. All the units are a.u.

Table S2 Topological parameters at the BCPs for the oxidation state of the IM1-PT11 spin adduct ^a

Complexes	BCP	ρ_{bcp}	$\nabla^2\rho_{\text{bcp}}$	V_{bcp}	G_{bcp}	H_{bcp}
IM1-PT11-CH	C5 - C15	0.2818	-0.7215	-0.3550	0.0873	-0.2677
	O12 - C14	0.0146	0.0594	-0.0110	0.0129	0.0019
	H8 - O30	0.2907	-1.8100	-0.6064	0.0769	-0.5294
	H8 - O11	0.0855	0.1559	-0.0972	0.0681	-0.0291
IM1-PT11-OH	C5 - C14	0.2517	-0.5830	-0.2767	0.0655	-0.2112
	O10 - N29	0.0416	0.1318	-0.0275	0.0302	0.0028
	O10 - H28	0.0123	0.0498	-0.0083	0.0104	0.0021

^a The ρ_{bcp} , $\nabla^2\rho_{\text{bcp}}$, V_{bcp} , G_{bcp} , and H_{bcp} is electron density, the Laplacian of the electron density, potential energy density, kinetic energy density, and energy density at the BCP, respectively. All the units are a.u.

Table S3 The Cartesian coordinates of the geometries including reactants, transition states, spin adducts, and the oxidated keto-enol tautomerization products

CBQ				DMPO			
C	0.00000000	1.02196700	0.00000000	C	-0.67911500	-1.34691700	-0.35628400
C	1.20240800	0.41768200	0.00000000	C	-1.94054100	-0.51934700	-0.00862000
C	1.35891700	-1.05129500	0.00000000	C	-1.42813700	0.88333200	-0.02331800
C	0.06848600	-1.90503300	0.00000000	C	0.51983800	-0.44077600	-0.01194400
C	-1.18835200	-1.19685900	0.00000000	H	-0.67326800	-1.57303500	-1.42513600
C	-1.29615500	0.25628300	0.00000000	H	-2.34568100	-0.78143000	0.97785800
H	2.12200800	0.99100400	0.00000000	H	-2.74907100	-0.67724000	-0.72799700
H		-2.11105700	-1.76651900	H	-2.00053200	1.79887400	0.02033100
	0.00000000			H	-0.63759600	-2.29449200	0.18340000
Cl	-0.14433500	2.74305500	0.00000000	C	1.06173400	-0.66334200	1.40423200
O	2.44684200	-1.57791400	0.00000000	H	1.58723200	-1.62040400	1.45412300
O	0.13027200	-3.12650100	0.00000000	H	1.75973200	0.13341000	1.66739100
O	-2.38074900	0.81530400	0.00000000	H	0.25528900	-0.67526900	2.14249200
				C	1.63805900	-0.46868800	-1.04807300
				H	2.40060700	0.27197600	-0.80484700
				H	2.09772900	-1.46057700	-1.06512600
				H	1.25253900	-0.24910700	-2.04672300
				N	-0.12544800	0.94908700	-0.02720700
				O	0.61251700	1.97726300	0.00984000
IM1(C5)				IM2(O11)			
C	2.29707600	-0.14577800	-0.23299400	C	-3.40820400	0.00652600	0.12728600
C	1.92712700	0.78739100	-1.13145700	C	-2.98255900	1.25612500	0.35156300
C	0.83146300	1.73400800	-0.89168800	C	-1.56477400	1.62971700	0.17899900
C	0.26564100	1.78410900	0.54548300	C	-0.61344100	0.53901800	-0.25254400
C	0.39694000	0.53052400	1.39281700	C	-1.04762700	-0.72391200	-0.44848100
C	1.63877700	-0.31524200	1.10459800	C	-2.46162400	-1.08907900	-0.30361300
H	2.42437800	0.86758000	-2.09098100	H	-3.64696600	2.05208700	0.66360000
H	0.46993700	0.83941500	2.43878800	H	-0.37814000	-1.53990500	-0.68833200
Cl	3.59843400	-1.23173200	-0.56950500	Cl	-5.07113400	-0.43936800	0.31632300
O	0.40055000	2.47266700	-1.75112100	O	-1.18175200	2.76533100	0.37652200
O	-0.25106300	2.79025700	0.96292100	O	0.63679700	1.00353400	-0.39471000
O	2.07041300	-1.07018000	1.94196900	O	-2.86122000	-2.21728000	-0.51430200
C	-2.95827800	0.50101700	0.31145800	C	3.64996600	1.17196300	-0.07683500
C	-2.21443800	0.32943300	1.65567400	C	2.80905200	1.15043200	-1.36961800
C	-0.88591600	-0.36647000	1.30527900	C	1.66250600	0.20773800	-1.03616000
C	-2.49796500	-0.67184500	-0.57342400	C	3.56744500	-0.26512200	0.48492500
H	-2.67703200	1.44753400	-0.15628200	H	3.21293300	1.87809600	0.63257300
H	-2.78200000	-0.30974500	2.33486400	H	3.37736700	0.73050800	-2.20342000
H	-2.06058100	1.28574000	2.15509900	H	2.44169000	2.13338100	-1.66243300
H	-0.68324700	-1.22333300	1.95497500	H	1.21904200	-0.32816400	-1.87711800
H	-4.04146100	0.50785300	0.44257800	H	4.68214300	1.47454900	-0.25884700
C	-3.29868000	-1.96059100	-0.31541700	C	4.70264900	-1.16747100	-0.02227600
H	-4.31662800	-1.84885600	-0.69710200	H	5.64718100	-0.87316500	0.44181000

H	-2.82686800	-2.80318300	-0.82489300	H	4.49717000	-2.20827400	0.23460000
H	-3.35851900	-2.19543900	0.75058800	H	4.81645200	-1.09868000	-1.10730300
C	-2.45803200	-0.34574500	-2.06587900	C	3.46696400	-0.32087600	2.01145300
H	-2.00438000	-1.16822000	-2.62216900	H	3.30287100	-1.34801900	2.34353900
H	-3.47411400	-0.19444000	-2.43888200	H	4.39415600	0.04470900	2.46061900
H	-1.88320100	0.56260500	-2.25820800	H	2.64116700	0.29690100	2.37132300
N	-1.10153000	-0.86531900	-0.06488600	N	2.27743300	-0.74096200	-0.11752600
O	-0.28380600	-1.68470600	-0.58868000	O	1.82843300	-1.91763500	0.06078700
IM3(O12)				IM4(O10)			
C	1.87538200	1.11808000	0.03387900	C	3.08321000	-0.67724900	-0.07878000
C	3.07980600	0.70589200	0.46219500	C	1.75284900	-0.92765200	-0.15338500
C	3.49677900	-0.69769600	0.30398300	C	0.84345700	0.16428500	-0.03784800
C	2.50460800	-1.65267200	-0.42683600	C	1.30262900	1.59906500	0.09035800
C	1.21324800	-1.08996100	-0.82029500	C	2.68820700	1.77817300	0.18783100
C	0.88746000	0.19780900	-0.58336500	C	3.64463900	0.73073400	0.11082200
H	3.79480400	1.38802200	0.90371000	H	1.35145700	-1.92645300	-0.26631100
H	0.49926500	-1.75289900	-1.29133000	H	3.06725300	2.78656300	0.29330900
Cl	1.45597100	2.81135500	0.13141700	Cl	4.21220200	-1.96035000	-0.18296700
O	4.56852800	-1.10160100	0.69575700	O	-0.40208900	-0.17600300	-0.08382000
O	2.81299500	-2.80770300	-0.62956900	O	0.42093600	2.48779600	0.08087700
O	-0.30756800	0.68556100	-1.00503900	O	4.86735900	0.86691100	0.17531800
C	-3.35241500	0.24479800	-1.09128600	C	-3.17131000	0.17725500	-1.48536100
C	-2.54865400	1.52347800	-0.77226600	C	-2.20614700	1.28099600	-1.00544200
C	-1.33600200	1.01208900	-0.01350700	C	-1.59259000	0.71363900	0.25878600
C	-3.13889200	-0.68675500	0.12215400	C	-3.69331600	-0.50284300	-0.20011600
H	-2.95513700	-0.22378500	-1.99437800	H	-2.63232900	-0.55030300	-2.09738200
H	-3.11506000	2.19347000	-0.12066100	H	-2.74010900	2.19411700	-0.73022000
H	-2.25313600	2.08100000	-1.66038200	H	-1.44879200	1.56173300	-1.73422700
H	-0.91156000	1.68590200	0.72821500	H	-1.24746700	1.41817900	1.00405500
H	-4.41019200	0.45212400	-1.25961500	H	-3.98653400	0.57773300	-2.08934300
C	-4.19933800	-0.48971100	1.21726500	C	-4.98654600	0.13581900	0.32914200
H	-5.15962900	-0.89184000	0.88496800	H	-5.82324100	-0.11765400	-0.32647000
H	-3.89902400	-1.01322800	2.12702400	H	-5.20519600	-0.23715300	1.33169500
H	-4.33462900	0.56757200	1.45970700	H	-4.90588400	1.22477500	0.37817000
C	-3.01430600	-2.16520800	-0.25200200	C	-3.84477500	-2.02020900	-0.32569600
H	-2.74676400	-2.75865500	0.62434300	H	-4.11317100	-2.45688100	0.63803200
H	-3.96650700	-2.53289700	-0.64300700	H	-4.63201800	-2.25677800	-1.04603600
H	-2.24887400	-2.31383500	-1.01699600	H	-2.91405700	-2.48009300	-0.66579700
N	-1.82446300	-0.18333800	0.64276800	N	-2.58334200	-0.18945700	0.76384700
O	-1.20893800	-0.71519100	1.61952800	O	-2.53818000	-0.65341900	1.94414300
IM5(C2)				IM6(C1)			
C	1.97312500	-0.66800700	-0.21034100	C	0.59348900	-0.41113200	0.59510000
C	0.62327200	-0.39576100	-0.68713600	C	1.73621800	-1.27080200	0.19090100
C	0.40803600	1.08377400	-1.00620500	C	2.88648200	-0.77732600	-0.51317700
C	1.18448400	2.11138100	-0.16403700	C	3.06069400	0.74480700	-0.61237100
C	2.38434400	1.64906800	0.46080700	C	2.20000900	1.53493000	0.23459800

C	2.86014500	0.28209400	0.46873000	C	1.12723400	0.99895700	1.04146400
H	0.38273500	-0.98831400	-1.57603700	H	1.67448500	-2.34146300	0.34702800
H	3.01205500	2.38758300	0.94819400	H	2.39794700	2.59771700	0.31859400
Cl	2.53510500	-2.27336200	-0.34837600	Cl	-0.27067400	-1.20049100	1.98857900
O	-0.35836600	1.41774400	-1.87161300	O	3.70979800	-1.54637800	-1.00912500
O	0.75529700	3.25974700	-0.07740500	O	3.93178500	1.23335500	-1.31987500
O	3.92265900	-0.06982500	0.98774300	O	0.64872400	1.58859500	1.98945700
C	-1.96314600	0.78149300	1.29800800	C	-2.54200300	-1.40848300	-0.64617600
C	-0.73813200	-0.09706200	1.63847600	C	-1.08212900	-1.49837700	-1.14489900
C	-0.50259100	-0.93968600	0.38432300	C	-0.38639000	-0.22966000	-0.62071200
C	-2.83081700	-0.06693700	0.34674300	C	-2.86812400	0.09273100	-0.54640200
H	-1.65119700	1.70152500	0.79921000	H	-2.62825200	-1.87166700	0.33737300
H	-0.95699700	-0.76387300	2.47584400	H	-1.04400600	-1.49603100	-2.23612100
H	0.13409200	0.49226300	1.92451500	H	-0.59628000	-2.41157600	-0.80348300
H	-0.18074100	-1.96403200	0.57880600	H	0.22203500	0.26095700	-1.39172900
H	-2.51567900	1.06893200	2.19344300	H	-3.22988800	-1.92076300	-1.32051800
C	-3.82751500	-0.96410200	1.10176400	C	-3.42672900	0.66782000	-1.85970700
H	-4.61701500	-0.34619500	1.53596000	H	-4.43997900	0.29310100	-2.02287300
H	-4.28466500	-1.68008900	0.41602900	H	-3.46228900	1.75767300	-1.80850200
H	-3.34308400	-1.51970400	1.90895500	H	-2.81404900	0.38233400	-2.71899500
C	-3.53550900	0.73619100	-0.74626000	C	-3.76420900	0.45424100	0.63938900
H	-4.06091900	0.06839900	-1.43129800	H	-3.88658600	1.53640300	0.71014600
H	-4.26646200	1.40548800	-0.28576400	H	-4.74919300	-0.00012100	0.50642200
H	-2.82545400	1.33389100	-1.31892900	H	-3.33484800	0.09249900	1.57562900
N	-1.79176600	-0.97325900	-0.26433600	N	-1.50324000	0.67939000	-0.32629700
O	-2.01899900	-1.70898700	-1.25190200	O	-1.31433400	1.89784200	-0.10580600
IM2(O11)-TS				IM3(O12)-TS			
C	3.10644200	-0.34241100	-0.02628900	C	1.90700400	1.14044200	-0.01259600
C	2.28495500	-1.15968600	-0.70104600	C	3.05955600	0.64147200	0.45889800
C	0.94423200	-0.71979600	-1.13373000	C	3.38743300	-0.78865200	0.30695200
C	0.55020000	0.73694700	-0.88426400	C	2.35794600	-1.67838200	-0.44543400
C	1.43246600	1.53426500	-0.16382200	C	1.14289300	-1.03589300	-0.89995400
C	2.73151900	1.08266400	0.30680500	C	0.87505900	0.31529600	-0.72219600
H	2.55508500	-2.18157300	-0.93787000	H	3.79286300	1.26094300	0.95980500
H	1.17417200	2.56150500	0.06441900	H	0.41849600	-1.64819900	-1.42113900
Cl	4.66646500	-0.86991200	0.51295800	Cl	1.55359600	2.84298000	0.16127900
O	0.17270400	-1.49324300	-1.66926800	O	4.41619300	-1.25808500	0.74028400
O	-0.56260600	1.14066100	-1.34875200	O	2.59341500	-2.86275500	-0.61724400
O	3.49417900	1.80896700	0.92463900	O	-0.19644800	0.86826600	-1.16028100
C	-3.60125400	-0.18446300	-0.92244800	C	-3.41450400	0.20576600	-1.01944900
C	-3.30053200	1.33259500	-0.93939800	C	-2.76830900	1.56517200	-0.66321300
C	-2.17040200	1.45796500	0.01800900	C	-1.62907300	1.18075100	0.21517600
C	-3.11070600	-0.68769400	0.45208300	C	-3.03316100	-0.75382100	0.13084700
H	-3.02882400	-0.67093400	-1.71312400	H	-2.99426000	-0.15855800	-1.95796200
H	-4.14946600	1.93500200	-0.59165300	H	-3.45056600	2.22017500	-0.10806500
H	-3.01810200	1.70054700	-1.92645100	H	-2.41948200	2.11690400	-1.53639200

H	-1.66435600	2.36066300	0.31922900	H	-0.99403000	1.85968300	0.76223400
H	-4.65896300	-0.40254900	-1.07480800	H	-4.49618200	0.27806100	-1.13803600
C	-4.19209700	-0.61398200	1.54042700	C	-4.08240300	-0.79480400	1.25101800
H	-4.94804200	-1.38026600	1.35428700	H	-4.97683400	-1.31222200	0.89651000
H	-3.75396600	-0.79294300	2.52446800	H	-3.69182900	-1.33220500	2.11758600
H	-4.68872900	0.35994900	1.55438500	H	-4.37133200	0.21056100	1.56864300
C	-2.44616800	-2.05861800	0.42040600	C	-2.65739600	-2.15980800	-0.32587900
H	-2.01509200	-2.29889100	1.39394900	H	-2.26448400	-2.74448000	0.50716500
H	-3.19963000	-2.81360300	0.18124500	H	-3.54590300	-2.66238400	-0.71570300
H	-1.66296200	-2.09877700	-0.33682100	H	-1.90615800	-2.13184900	-1.11647100
N	-2.08109900	0.38536700	0.79654000	N	-1.81106800	-0.05171000	0.70115600
O	-1.23868400	0.23687600	1.72991600	O	-1.02618500	-0.61622100	1.52311300
IM4(O10)-TS				IM5(C2)-TS			
C	-3.17590900	0.66771100	-0.03939300	C	2.00701500	-0.64592800	-0.26025400
C	-1.87120100	0.99645200	-0.03478300	C	0.73595200	-0.36991100	-0.79714400
C	-0.87409300	-0.05616700	0.03314800	C	0.43641700	1.08222400	-1.05136600
C	-1.29374400	-1.53906200	0.11959200	C	1.15876700	2.11683400	-0.16825000
C	-2.66198800	-1.78693200	0.09955400	C	2.34217400	1.67194400	0.49749300
C	-3.66986600	-0.78233400	0.02288300	C	2.84439100	0.31431300	0.48847100
H	-1.52281700	2.02041000	-0.07914800	H	0.38796800	-1.02243200	-1.59674600
H	-3.00032900	-2.81446500	0.14386900	H	2.92159100	2.40591000	1.04686800
Cl	-4.38376900	1.89387200	-0.11957800	Cl	2.59411600	-2.25844000	-0.35576000
O	0.32338900	0.28631500	0.01249100	O	-0.35231100	1.41128400	-1.90377700
O	-0.36231500	-2.37239000	0.18508100	O	0.69330400	3.25108100	-0.07586900
O	-4.88056200	-0.98459300	0.00304900	O	3.88226000	-0.02926600	1.05319600
C	3.12297700	-0.04187600	-1.54489000	C	-1.95794600	0.78420000	1.29357500
C	2.31283800	-1.27574500	-1.08982300	C	-0.76671600	-0.12727900	1.67104100
C	1.91498600	-0.94482800	0.30328500	C	-0.59624400	-1.01904200	0.46552400
C	3.70033200	0.57748200	-0.25072000	C	-2.82663300	-0.05057500	0.33047400
H	2.45778300	0.67258700	-2.03261800	H	-1.60508900	1.68779700	0.79358200
H	2.92911300	-2.18377500	-1.04671300	H	-0.99151300	-0.74568800	2.54607100
H	1.45208000	-1.51488900	-1.71031700	H	0.13808700	0.43534700	1.91198700
H	1.38017100	-1.60411100	0.96974000	H	-0.14165100	-2.00040400	0.55314000
H	3.91304000	-0.30106700	-2.24992000	H	-2.52504100	1.09654600	2.17099900
C	5.11609600	0.08335300	0.07372100	C	-3.87782400	-0.89618800	1.06920600
H	5.82470600	0.51596000	-0.63600700	H	-4.65461800	-0.23769300	1.46414500
H	5.40545800	0.38930200	1.08110500	H	-4.34098800	-1.60849900	0.38396100
H	5.18768700	-1.00545600	0.00813500	H	-3.44095900	-1.45017100	1.90422700
C	3.60950300	2.10132700	-0.19685800	C	-3.45752700	0.73922700	-0.81300700
H	3.94465800	2.47479900	0.77236100	H	-3.98236500	0.06910600	-1.49620100
H	4.24845200	2.52915900	-0.97313600	H	-4.18068700	1.44633900	-0.39907300
H	2.58471800	2.43758200	-0.36552700	H	-2.70783200	1.29617700	-1.37513600
N	2.76435900	-0.01023300	0.79359800	N	-1.80095000	-1.03533100	-0.21062100
O	2.79314700	0.35360400	2.00206900	O	-2.05090100	-1.79940500	-1.16606400
IM6(C1)-TS				IM1-PT11			
C	-0.76150300	1.11999000	0.03625600	C	-2.90630100	-0.31499100	-0.05198500

C	-1.92211000	0.92476900	-0.78093400	C	-3.09068600	0.98298000	-0.30857200
C	-2.74500900	-0.25880500	-0.75020300	C	-1.96065900	1.92447200	-0.23136400
C	-2.47704600	-1.26945500	0.38180000	C	-0.59528700	1.38196600	0.15328000
C	-1.42409700	-0.93228700	1.32255300	C	-0.38846400	0.03653700	0.27901400
C	-0.61958200	0.25107500	1.27723400	C	-1.55038500	-0.87281600	0.29927900
H	-2.17337900	1.66981600	-1.52778900	H	-4.05257700	1.40305900	-0.57348000
H	-1.27082400	-1.59950000	2.16344600	H	1.08687300	2.04355200	0.79164600
Cl	-0.45277000	2.85283300	0.38160100	Cl	-4.21126400	-1.45406100	-0.10615300
O	-3.65063300	-0.44002900	-1.55354400	O	-2.10952900	3.10444300	-0.46949900
O	-3.13852500	-2.28738600	0.47923600	O	0.28253700	2.36006600	0.30863700
O	0.22638600	0.51574500	2.13065500	O	-1.43396200	-2.04969400	0.59891600
C	2.87343100	0.67224900	0.08870500	C	2.45179800	-1.20154900	-1.32824000
C	2.01839800	1.41605300	-0.95811100	C	1.28007500	-1.78413500	-0.51606700
C	0.75384800	0.58775900	-1.06608300	C	0.92535400	-0.70244400	0.54112700
C	2.50724100	-0.81334200	-0.07277500	C	3.24307200	-0.32975100	-0.34068400
H	2.60411400	1.00823700	1.09090600	H	2.07363100	-0.57493700	-2.14112400
H	2.50509400	1.44026600	-1.93898700	H	1.57531300	-2.70052400	-0.00324500
H	1.81453900	2.44626900	-0.67486700	H	0.43055700	-2.03449300	-1.14605900
H	0.21909200	0.58335200	-2.00779700	H	0.85056100	-1.15792700	1.53435600
H	3.94121000	0.83772700	-0.06009500	H	3.07382700	-1.98053600	-1.77242300
C	3.33035900	-1.50768300	-1.17480600	C	4.24065800	-1.13913500	0.50773600
H	4.36104500	-1.61919200	-0.83103900	H	5.07369400	-1.47055400	-0.11719700
H	2.92584500	-2.49964600	-1.38561400	H	4.63721500	-0.51797700	1.31344100
H	3.34048900	-0.93180100	-2.10344200	H	3.77464800	-2.02211600	0.95177000
C	2.52166900	-1.62746400	1.21636200	C	3.93003700	0.87269100	-0.98885200
H	2.12990400	-2.63178900	1.04515000	H	4.39828700	1.50404400	-0.23222800
H	3.55481800	-1.71764400	1.56070800	H	4.70272900	0.52453300	-1.67877200
H	1.93515000	-1.14101800	1.99564700	H	3.21458500	1.47838300	-1.54979500
N	1.09549600	-0.69825000	-0.62793100	N	2.13639100	0.14589500	0.54170600
O	0.28876400	-1.64241000	-0.62358500	O	2.30122200	1.09522400	1.38041300
IM1-PT12				IM2-PT11			
C	-2.69416700	-0.50330800	0.04699200	C	-3.66240500	0.17386200	0.11661000
C	-3.17373200	0.72500200	0.29234800	C	-2.90835700	1.28421700	0.11265300
C	-2.27544700	1.88425900	0.24433300	C	-1.42401500	1.21192000	0.06944800
C	-0.76353800	1.62575700	-0.05313000	C	-0.95830100	-0.17777900	0.06443700
C	-0.36629200	0.27238200	-0.43170800	C	-1.59446800	-1.30435600	0.16299300
C	-1.26443700	-0.75608600	-0.26786300	C	-3.04014200	-1.20269600	-0.11558700
H	-4.21612300	0.90325900	0.52238400	H	-3.33406900	2.27894400	0.15272600
H	0.02705000	-2.18369000	-0.21386900	H	0.60417700	-1.17568200	0.85837300
Cl	-3.74402000	-1.88651700	0.09316000	Cl	-5.39624300	0.25490500	0.18609500
O	-2.66954900	3.01532700	0.42121100	O	-0.72565400	2.21200200	0.11167700
O	0.00345700	2.56539900	0.05583700	O	0.62042200	-0.27149100	0.47456100
O	-0.95255600	-2.03744700	-0.38731800	O	-3.70600600	-2.08618700	-0.60937000
C	2.92914800	1.24606200	-0.20853000	C	3.20361700	1.45568200	-0.16055700
C	1.97613300	1.06747800	-1.40577900	C	2.02836700	1.07792500	-1.08691800
C	1.01898100	-0.06495600	-0.98651600	C	1.64764300	-0.31855000	-0.64886000

C	3.13337500	-0.16707300	0.37737300	C	3.94736100	0.13531200	0.13667400
H	2.45833100	1.89644300	0.53083000	H	2.81478000	1.88231400	0.76656900
H	2.52921700	0.73189900	-2.28707800	H	2.34122000	1.02694800	-2.13336400
H	1.46200700	1.99030600	-1.65597900	H	1.19105700	1.76890400	-1.00708200
H	0.85320600	-0.74876200	-1.82699200	H	1.21134000	-0.98397300	-1.39294600
H	3.87912800	1.69630500	-0.50177700	H	3.86136800	2.19549800	-0.61810200
C	4.28907700	-0.93014100	-0.29294600	C	5.06675900	-0.16263300	-0.87263800
H	5.24302300	-0.48897400	0.00591500	H	5.90087800	0.52565500	-0.71609200
H	4.27865400	-1.97799300	0.01307300	H	5.43131400	-1.18367600	-0.74166300
H	4.21882800	-0.88880600	-1.38272100	H	4.71950300	-0.05140500	-1.90303200
C	3.27719100	-0.18831500	1.90157200	C	4.45973300	0.02889000	1.57350400
H	3.31481600	-1.21551300	2.26958000	H	4.87885200	-0.96129800	1.76010100
H	4.20077700	0.31874800	2.19192500	H	5.24071500	0.77457500	1.74105800
H	2.43901000	0.32355500	2.37940100	H	3.65512800	0.20539300	2.29088300
N	1.84673300	-0.81509100	-0.00912200	N	2.84363300	-0.86507100	-0.07625300
O	1.55809100	-2.02411900	0.30259100	O	2.90119800	-2.07818100	0.29840400
IM2-PT12				IM3-PT11			
C	-3.18525500	0.04505800	0.32686900	C	1.70941800	1.20696800	0.03925600
C	-2.68681400	1.27982400	0.49179900	C	2.62066400	0.61792400	0.82856100
C	-1.40808600	1.67544100	-0.16339500	C	2.96612700	-0.82868300	0.65886400
C	-0.62101700	0.50179700	-0.74453900	C	2.45534500	-1.41705800	-0.64370900
C	-1.22655800	-0.67310000	-1.02506700	C	1.42716400	-0.82773000	-1.27083000
C	-2.51868600	-0.84529800	-0.65311400	C	0.89956300	0.34303400	-0.85723200
H	-3.18668500	2.03927300	1.07776900	H	3.16285600	1.15260200	1.59705000
H	-2.82199300	-2.19060400	-1.91147800	H	2.91163800	-2.62474500	-2.01222200
Cl	-4.69077700	-0.44729800	1.05732100	Cl	1.38783500	2.93340500	0.15846300
O	-0.98227500	2.80698600	-0.09911700	O	3.75005200	-1.38693700	1.39268700
O	0.68455900	0.77734300	-0.81215600	O	3.23897200	-2.39598600	-1.13056300
O	-3.34457600	-1.71915300	-1.24416100	O	-0.37653400	0.67062800	-1.17203800
C	3.73542000	0.76421600	-0.62140000	C	-3.33708800	0.02200400	-1.04428400
C	2.83593300	0.20760900	-1.74435300	C	-2.64616000	1.39014400	-0.85702100
C	1.61518600	-0.32154300	-1.01074500	C	-1.34971700	1.04704700	-0.14613100
C	3.50833300	-0.17011500	0.58765000	C	-2.95052300	-0.81381600	0.19854800
H	3.42032900	1.77924700	-0.36945600	H	-2.95606800	-0.45953000	-1.94697400
H	3.31977500	-0.62372100	-2.26423000	H	-3.23586000	2.04877600	-0.21420700
H	2.56074400	0.95769700	-2.48544500	H	-2.45744100	1.90946100	-1.79610200
H	1.06830100	-1.14288100	-1.47430900	H	-0.93092500	1.81933800	0.49389800
H	4.78661700	0.80171100	-0.91187900	H	-4.41935700	0.11697200	-1.14506300
C	4.51475500	-1.33004400	0.64188300	C	-3.98581000	-0.71275700	1.32917600
H	5.50457800	-0.95668600	0.91715900	H	-4.89520600	-1.25276800	1.05342400
H	4.19987300	-2.06279200	1.38777000	H	-3.58549100	-1.15264900	2.24499000
H	4.59457600	-1.83691100	-0.32347100	H	-4.25260500	0.32716400	1.53604800
C	3.45793700	0.57033400	1.92637400	C	-2.63279300	-2.27563700	-0.12567800
H	3.19468900	-0.11795700	2.73164300	H	-2.27690900	-2.79482900	0.76607900
H	4.43544500	1.00767700	2.14661000	H	-3.53348800	-2.77965900	-0.48622200
H	2.71653600	1.37192000	1.90055800	H	-1.86121200	-2.34406500	-0.89537300

N	2.15325000	-0.73647200	0.27567500	N	-1.69978800	-0.11406000	0.64564400
O	1.48614100	-1.42663600	1.10578400	O	-0.91520900	-0.58072600	1.52668700
IM3-PT12				IM1-PT11-1W			
C	1.79854300	1.12898100	0.07326300	C	2.95719200	-0.54609900	-0.07373600
C	2.83755100	0.57530800	0.72369000	C	3.04712400	0.78498900	-0.17972700
C	3.12802500	-0.86968500	0.54140400	C	1.84859600	1.61980000	-0.05172900
C	2.44691900	-1.54410500	-0.71016700	C	0.52833100	0.94853300	0.19672300
C	1.15660900	-0.97359700	-1.13676300	C	0.42819400	-0.40463600	0.27995000
C	1.00185900	0.26614900	-0.77278800	C	1.63543100	-1.24298600	0.17986600
H	3.47101500	1.13782000	1.39614500	H	3.98155100	1.30120000	-0.35899300
H	-0.57595200	0.12832900	-1.87763000	H	0.60322900	4.46091800	-0.12131500
Cl	1.42663900	2.84217900	0.23240300	Cl	4.34702300	-1.56320400	-0.21121900
O	3.89150600	-1.47475600	1.25789200	O	1.91753900	2.83910000	-0.14554500
O	3.06121900	-2.40715200	-1.29586200	O	-0.54421900	1.72202400	0.32614200
O	-0.37405700	0.88717400	-1.28419300	O	1.60711300	-2.45272000	0.30284800
C	-3.25425100	-0.40315200	-1.08612200	C	-2.99230600	-0.13222800	1.30715600
C	-2.84913800	1.08661300	-1.15926000	C	-1.68814800	-0.83557700	1.75157300
C	-1.58261500	1.15120100	-0.33003600	C	-0.88993700	-1.12540500	0.45466200
C	-2.82013100	-0.87699500	0.32044900	C	-3.24131400	-0.57248000	-0.14521200
H	-2.73043200	-0.98184200	-1.85288300	H	-2.85610900	0.94928100	1.33853300
H	-3.59776100	1.72374100	-0.68088400	H	-1.90357500	-1.77952000	2.25597900
H	-2.70431400	1.45973600	-2.17382000	H	-1.12175300	-0.21790300	2.44847200
H	-1.29301000	2.09438700	0.11969400	H	-0.66927100	-2.19184500	0.37155200
H	-4.32284500	-0.54331600	-1.25029600	H	-3.83345400	-0.38808100	1.95466800
C	-3.92880500	-0.70980700	1.36951500	C	-4.00190100	-1.90855600	-0.23477100
H	-4.71258600	-1.45229200	1.20222000	H	-5.03960900	-1.77413600	0.08266100
H	-3.52015300	-0.85776500	2.37075800	H	-3.99642800	-2.27326400	-1.26413900
H	-4.38148000	0.28471700	1.32657100	H	-3.54832700	-2.67372800	0.40138500
C	-2.24361200	-2.29365100	0.34163900	C	-3.91834500	0.49676200	-1.00189400
H	-1.88951200	-2.54260100	1.34369300	H	-3.97256800	0.17125200	-2.04238400
H	-3.01860600	-3.01146900	0.06080300	H	-4.93325700	0.68018100	-0.63897300
H	-1.40450600	-2.38844600	-0.35130900	H	-3.35738600	1.43276400	-0.96131500
N	-1.72826800	0.11468400	0.63094200	N	-1.84424000	-0.78031500	-0.62883900
O	-1.03123800	0.07043500	1.69098200	O	-1.57553500	-1.02285800	-1.84563500
IM1-PT12-1W				IM1-PT11-2W			
C	2.91141600	-0.03118500	0.03294400	C	2.57891000	-1.55275300	-0.06005400
C	3.08277700	1.26867500	-0.25072400	C	2.98315600	-0.28105800	-0.16526000
C	1.92108800	2.15715100	-0.34443400	C	2.01429200	0.81008900	-0.03768700
C	0.52080800	1.53655900	-0.05860000	C	0.57288700	0.47463000	0.20884400
C	0.43848000	0.11895800	0.28887300	C	0.15418400	-0.81781900	0.29155400
C	1.57304300	-0.65311000	0.24898800	C	1.12754000	-1.91673600	0.19228700
H	4.06208400	1.69752000	-0.41895700	H	4.01412100	-0.00310400	-0.34302900
H	-0.10322300	-3.95846800	-1.28508300	H	1.04185700	4.50173800	0.07687200

Cl	4.29087900	-1.08438200	0.14535000	Cl	3.68791700	-2.86978800	-0.19629000
O	2.02085700	3.33259500	-0.61860300	O	2.35630700	1.98268700	-0.12676700
O	-0.45513600	2.26059200	-0.13468100	O	-0.27630600	1.48196800	0.33708900
O	1.63097500	-1.96565500	0.41939400	O	0.81720700	-3.08668600	0.31487500
C	-2.86678700	0.99997200	1.22707600	C	-3.09741100	0.28673700	1.27690300
C	-1.63293400	0.31346200	1.85456100	C	-2.01827000	-0.71856800	1.74304300
C	-0.90785500	-0.44209700	0.71051900	C	-1.29843700	-1.20567600	0.46025700
C	-3.22800300	0.18721000	-0.03014000	C	-3.43501100	-0.09171500	-0.17543000
H	-2.61474900	2.01980500	0.94354600	H	-2.69181400	1.29849600	1.30062800
H	-1.93405500	-0.41194400	2.61352100	H	-2.47170000	-1.57578900	2.24457600
H	-0.97778200	1.03645000	2.33874600	H	-1.32552100	-0.25979000	2.44858800
H	-0.76723900	-1.48385000	1.00457000	H	-1.33483300	-2.29497200	0.39046800
H	-3.70588500	1.03189400	1.92488900	H	-3.98288600	0.25845300	1.91533900
C	-4.23336200	-0.94030200	0.26810000	C	-4.51466500	-1.18631800	-0.26358100
H	-5.20862600	-0.50896000	0.50692500	H	-5.48606800	-0.78234300	0.03458500
H	-4.34289800	-1.59028400	-0.60208800	H	-4.58946200	-1.55406100	-1.28908500
H	-3.91373300	-1.55123800	1.11719800	H	-4.28453000	-2.03422900	0.38768700
C	-3.70376400	1.05270200	-1.19896400	C	-3.80206400	1.10612100	-1.05109500
H	-3.85443800	0.44146100	-2.09092400	H	-3.92970100	0.79218100	-2.08876100
H	-4.65267800	1.53014900	-0.94098100	H	-4.73825100	1.55099000	-0.70293100
H	-2.97027300	1.82934300	-1.42140900	H	-3.01691800	1.86388400	-1.01428200
N	-1.91722600	-0.43838300	-0.38208300	N	-2.13431500	-0.65990000	-0.63844200
O	-1.80199200	-1.19318300	-1.40602300	O	-1.93052700	-0.99131900	-1.84678900
O	-0.35682200	-3.29732500	-0.63374200	O	0.14636000	4.11698000	0.17178100
H	-0.91369800	-2.61957200	-1.09216200	H	-0.32118200	4.65460100	0.81728500
H	0.82031900	-2.46328900	0.10590300	H	0.11424300	2.39190000	0.23804600
				O	2.81442300	4.76295100	-0.10863900
				H	3.22045800	5.20402100	-0.86083000
				H	3.01742000	3.81945300	-0.20021300
IM1-PT12-2W				IM1-PT11-TS			
C	-2.80918400	-0.64076600	0.12640100	C	-2.51143200	-0.15824900	0.18873600
C	-2.85978700	-1.87343000	-0.39922300	C	-2.33296100	1.03400000	0.79406600
C	-1.61837600	-2.60626500	-0.66540800	C	-1.18937400	1.90227900	0.47927200
C	-0.27977800	-1.91497400	-0.26860100	C	-0.44567200	1.43475300	-0.74338900
C	-0.32904000	-0.58695100	0.33618200	C	-0.36177300	0.06845000	-1.15849800
C	-1.53417900	0.06407600	0.45084900	C	-1.52894800	-0.77314100	-0.80455000
H	-3.79563100	-2.35964800	-0.64193200	H	-3.02781300	1.40466600	1.53789800
H	-0.32706800	3.78905000	-0.28560900	H	-0.00880100	1.06468200	-2.23469300
Cl	-4.28555400	0.22593400	0.44451600	Cl	-3.88889900	-1.12950500	0.56496900
O	-1.61095700	-3.71173400	-1.16075000	O	-0.87785800	2.89488500	1.10285600
O	0.75928300	-2.51566300	-0.47805900	O	0.03736000	2.20512800	-1.63326600
O	-1.71543800	1.30486400	0.86497100	O	-1.72685900	-1.87562800	-1.26673400
C	3.09387600	-1.24563900	1.03614100	C	3.03031400	0.54462700	-0.60017000
C	1.81029200	-0.84905800	1.80013700	C	2.25437800	-0.12993200	-1.74818600
C	0.96598600	0.02484500	0.83683900	C	0.98463500	-0.70928600	-1.09936500
C	3.31364800	-0.16412000	-0.03715400	C	2.75644700	-0.32468800	0.64291000

H	2.95058100	-2.21235900	0.55725600	H	2.65343600	1.55754000	-0.43348300
H	2.05091600	-0.25714800	2.68613000	H	2.83652300	-0.95617300	-2.16351700
H	1.26053200	-1.72743500	2.13561400	H	2.04590700	0.55718300	-2.56719500
H	0.72867600	0.96997000	1.32794700	H	0.72736700	-1.68671900	-1.51282900
H	3.95491700	-1.31378500	1.70410500	H	4.09762300	0.62230100	-0.81458000
C	4.17613100	1.00441200	0.47464900	C	3.75276500	-1.48877000	0.78067400
H	5.20707700	0.66906800	0.61347600	H	4.74048000	-1.10757500	1.05366500
H	4.16917000	1.82372800	-0.24690800	H	3.41925300	-2.17701000	1.56023100
H	3.80951500	1.38546800	1.43211400	H	3.84800400	-2.05001300	-0.15236800
C	3.86227800	-0.71567400	-1.35469900	C	2.67576500	0.47627600	1.94315300
H	3.90628300	0.07189000	-2.10953700	H	2.37329500	-0.16726500	2.77057000
H	4.87156800	-1.10634300	-1.20005500	H	3.65470900	0.90494200	2.17248300
H	3.22758400	-1.52312100	-1.72384800	H	1.95478000	1.29320000	1.86232600
N	1.92497000	0.34105800	-0.25584300	N	1.40817000	-0.89090300	0.30910000
O	1.68169800	1.24945400	-1.11826800	O	0.62166600	-1.35935600	1.18531800
O	-1.16679800	5.25123100	-1.04935900				
H	-1.06248800	6.13365200	-0.67888600				
H	-2.08741500	5.18333400	-1.32324900				
O	0.06050400	3.01685500	0.16425900				
H	-0.95866500	1.94942500	0.65546600				
H	0.65655100	2.55718900	-0.46697600				
IM1-PT12-TS				IM2-PT11-TS			
C	2.39914400	-0.35350400	-0.22846000	C	-3.60332800	0.11576700	0.00525400
C	2.40517500	0.81970300	-0.88733700	C	-2.95520600	1.29227400	0.02107000
C	1.49233100	1.93409600	-0.52089300	C	-1.47720100	1.36982300	0.13511200
C	0.34984100	1.67214500	0.52829400	C	-0.86538000	0.04285000	0.19224000
C	0.35045900	0.34878200	1.17038800	C	-1.40455200	-1.16764300	0.20663100
C	1.51383500	-0.47515500	0.92313400	C	-2.88453500	-1.23283700	0.09711300
H	3.12431700	1.02770700	-1.67052100	H	-3.47610000	2.23933700	-0.04570300
H	0.88849000	-0.32785100	2.39387600	H	0.19331100	-1.27441600	0.43848900
Cl	3.50665400	-1.63934700	-0.55903200	Cl	-5.33487000	0.05621900	-0.13027400
O	1.59761900	3.01542400	-1.05010500	O	-0.88124200	2.43534700	0.18034600
O	-0.46984500	2.54731500	0.70813700	O	0.57749000	-0.18861000	0.43754400
O	1.76219700	-1.17604700	1.95877000	O	-3.51834000	-2.26281400	0.07432400
C	-3.06231900	0.61910900	0.43065000	C	3.31900100	1.34394400	0.46959100
C	-2.24241300	0.25647200	1.68988600	C	2.14371600	1.51228100	-0.51605900
C	-0.97859200	-0.45540100	1.17151800	C	1.58937300	0.10967900	-0.66026700
C	-2.72100600	-0.44803300	-0.62911500	C	3.90580500	-0.05430400	0.17949700
H	-2.76074800	1.60474000	0.07306700	H	2.94818600	1.38623700	1.49622500
H	-2.79771000	-0.43369400	2.32946300	H	2.49536500	1.83579300	-1.50030000
H	-2.00160100	1.14088800	2.27507600	H	1.38365700	2.21559500	-0.18049600
H	-0.79979600	-1.38995900	1.71008100	H	1.08522400	-0.14566700	-1.59211800
H	-4.13373100	0.64846900	0.63687400	H	4.06693900	2.12909500	0.35296800
C	-3.61224200	-1.69843500	-0.52045400	C	5.02194800	-0.02869400	-0.87559400
H	-4.62893900	-1.45969300	-0.84327900	H	5.92030400	0.43113300	-0.45665000
H	-3.22341600	-2.49575100	-1.15751200	H	5.26676100	-1.04574400	-1.18853500

H	-3.65902200	-2.07048800	0.50643400	H	4.72604600	0.54052000	-1.76062600
C	-2.70662000	0.08824100	-2.06075900	C	4.35413200	-0.80478100	1.43483400
H	-2.34829300	-0.67596500	-2.75303100	H	4.65820400	-1.82256200	1.18389400
H	-3.71782300	0.37923400	-2.35607900	H	5.20400200	-0.28993800	1.88998800
H	-2.06006800	0.96455500	-2.14505600	H	3.54719300	-0.85584500	2.16930200
N	-1.33291200	-0.81924500	-0.21585300	N	2.71090400	-0.74783500	-0.41466700
O	-0.55121600	-1.53127900	-0.91505100	O	2.67643400	-1.99074700	-0.67041800
IM2-PT12-TS				IM3-PT11-TS			
C	-3.60240900	0.16990600	0.00910600	C	1.80128700	1.10630900	0.04176200
C	-3.00257000	1.36506400	-0.08138600	C	2.98660600	0.67482200	0.51775700
C	-1.51162900	1.48429700	-0.12783800	C	3.40516300	-0.72003600	0.32531200
C	-0.69831100	0.20258900	-0.02536300	C	2.38583500	-1.53749300	-0.44710100
C	-1.31482700	-1.00597100	0.04321800	C	1.15535800	-1.06620800	-0.95246100
C	-2.73186200	-1.00897300	0.06528900	C	0.81863000	0.21870100	-0.66348800
H	-3.55182000	2.29618900	-0.13424700	H	3.68329500	1.34141600	1.00745900
H	-1.91551600	-2.42058700	0.13806000	H	1.37524200	-2.57370700	-1.20543100
Cl	-5.32631900	-0.03266300	0.06006800	Cl	1.42749600	2.81256100	0.16463900
O	-0.99643700	2.57270700	-0.25826300	O	4.45821300	-1.17762400	0.71628200
O	0.61001400	0.44247100	-0.02674900	O	2.47567800	-2.78597100	-0.68779800
O	-3.13116400	-2.22029000	0.14443000	O	-0.34738800	0.74489300	-1.10185100
C	3.21245100	-0.21738600	-1.52110200	C	-3.29650800	-0.01359700	-1.10543400
C	2.02691000	-1.16159400	-1.23346400	C	-2.65855600	1.38654200	-0.97477200
C	1.51649500	-0.69335200	0.12324500	C	-1.40219200	1.13532000	-0.16164400
C	3.86180300	0.05520000	-0.14520400	C	-2.97405000	-0.74389300	0.21913600
H	2.84387200	0.71801600	-1.94838900	H	-2.83969900	-0.54699400	-1.94126100
H	2.35850900	-2.19966600	-1.14269900	H	-3.30702100	2.07026200	-0.42087000
H	1.24757600	-1.12515300	-1.99430900	H	-2.42219300	1.84274800	-1.93555100
H	1.01873400	-1.44342600	0.73482900	H	-1.04707500	1.95956900	0.45291900
H	3.92502500	-0.64927700	-2.22553600	H	-4.37140700	0.03767000	-1.28526400
C	4.98580000	-0.93756000	0.18906700	C	-4.07691200	-0.57415300	1.27570100
H	5.86176800	-0.73719300	-0.43327500	H	-4.95895100	-1.15277300	0.98986100
H	5.27351800	-0.83643600	1.23748200	H	-3.72650700	-0.93337800	2.24558900
H	4.67175700	-1.97085600	0.01865600	H	-4.37227800	0.47295800	1.38320500
C	4.33853400	1.49960200	0.02815600	C	-2.61606500	-2.21968400	0.03140200
H	4.69514500	1.66091200	1.04730100	H	-2.31623900	-2.66344800	0.98263600
H	5.15794100	1.70833200	-0.66493800	H	-3.48526400	-2.76400300	-0.34737700
H	3.52663800	2.20314100	-0.16814300	H	-1.79303600	-2.33378400	-0.67669800
N	2.70856800	-0.20354900	0.77777300	N	-1.76419800	0.01692500	0.68099600
O	2.76658400	-0.01174000	2.03149600	O	-1.02506400	-0.35233900	1.64185900
IM3-PT12-TS				IM1-PT11-1W			
C	1.82050800	1.15236800	0.05311900	C	-2.86373700	-0.16584400	0.27041400
C	2.93910700	0.63736200	0.59442100	C	-2.77848600	1.15590400	0.48211100
C	3.25799100	-0.80039000	0.42006400	C	-1.53584200	1.89635800	0.21286700
C	2.35815600	-1.64505200	-0.57720600	C	-0.40714800	1.11023100	-0.45247400
C	1.09546500	-1.01857000	-1.01640300	C	-0.42926800	-0.32589200	-0.50769600
C	0.95328200	0.25606400	-0.67951100	C	-1.66763300	-1.01762400	-0.09553900

H	3.63221500	1.23557600	1.17089000	H	-3.61949900	1.73969000	0.83605000
H	-0.28843000	-0.37355900	-1.67142000	H	-0.18113200	-0.26825500	-2.03063800
Cl	1.42704600	2.85408700	0.19424600	Cl	-4.35634800	-1.01463300	0.51684200
O	4.18655000	-1.31893000	0.99701300	O	-1.42192600	3.08102100	0.44026700
O	2.76255200	-2.72708500	-0.93405900	O	0.46774800	1.77594500	-1.07513100
O	-0.31606700	0.68722400	-1.31897000	O	-1.75045600	-2.23099100	-0.02511400
C	-3.20967500	-0.52474200	-1.09807400	C	3.12300300	-0.63237900	-0.91733500
C	-2.76386400	0.93055600	-1.36282000	C	1.93751900	-1.60986600	-1.04533100
C	-1.54219700	1.09757700	-0.48217800	C	0.85976300	-1.09392300	-0.06442500
C	-2.86098200	-0.79966100	0.38286700	C	3.10744900	-0.15200300	0.54654100
H	-2.65802000	-1.21266700	-1.74442400	H	2.98469000	0.22472300	-1.58068600
H	-3.52260800	1.64402600	-1.03118700	H	2.23829300	-2.60996300	-0.72444600
H	-2.54627200	1.14060200	-2.41015700	H	1.58163200	-1.69765900	-2.06875500
H	-1.27991300	2.09447000	-0.14285200	H	0.45924500	-1.93999100	0.49721300
H	-4.27181200	-0.66932500	-1.29737200	H	4.07269400	-1.10233400	-1.17997500
C	-4.01456300	-0.46120400	1.33837300	C	3.88054100	-1.09542100	1.48553700
H	-4.81021700	-1.20294000	1.23639200	H	4.95399700	-1.01898400	1.29253700
H	-3.65988600	-0.47346900	2.37070200	H	3.69622700	-0.82177500	2.52668400
H	-4.43585500	0.52644900	1.13206500	H	3.58147600	-2.13773100	1.34760600
C	-2.33066600	-2.21193500	0.63681400	C	3.57283900	1.29339300	0.72302600
H	-2.02739700	-2.32099900	1.67970800	H	3.46696300	1.60575400	1.76307100
H	-3.11568200	-2.94289600	0.42672000	H	4.62506800	1.37654700	0.43806000
H	-1.46872900	-2.43000000	0.00259800	H	2.98385400	1.97074100	0.10198900
N	-1.75765000	0.20104100	0.60724300	N	1.64839200	-0.25441700	0.86393000
O	-1.09790900	0.28175700	1.68959800	O	1.09652100	0.39430200	1.79781400
				O	0.41059800	0.22182100	-2.89962300
				H	-0.18698400	0.53744100	-3.59095300
				H	0.64877200	1.05708400	-2.19346200
IM1-PT12-1W				IM1-PT11-2W			
C	-2.53657800	0.05457700	-0.55559500	C	2.65305000	-0.92593100	-0.19278900
C	-2.64788200	-1.28209100	-0.50664700	C	2.85129000	0.05371300	-1.08667000
C	-1.67796800	-2.09639600	0.24821000	C	1.84203300	1.10096400	-1.28072000
C	-0.36484900	-1.39915900	0.70429500	C	0.46457600	0.93159700	-0.59144800
C	-0.35263700	0.06327800	0.75510600	C	0.32873500	-0.05611300	0.41959200
C	-1.47080400	0.78429500	0.18967300	C	1.39303800	-1.04692000	0.64473200
H	-3.47359100	-1.80559700	-0.97314500	H	3.76664300	0.14064300	-1.65957500
H	-0.63286800	0.74393700	2.14814600	H	0.65892700	2.97129000	1.38804200
Cl	-3.70276000	1.02794600	-1.39233000	Cl	3.86987500	-2.12772500	0.09231800
O	-1.87040600	-3.26987200	0.47504300	O	2.06338600	2.09110700	-1.94969300
O	0.58738500	-2.10425100	0.98428500	O	-0.41200600	1.77562800	-0.87575700
O	-1.64105300	2.01301100	0.42203400	O	1.32642700	-1.92215100	1.49188100
C	3.21236000	-0.37369500	0.79620700	C	-3.19647400	0.66758400	0.42072400
C	2.15051900	0.42470000	1.58929700	C	-2.06437200	0.52592500	1.46260900
C	1.01713900	0.75247200	0.58882600	C	-1.05947000	-0.49768200	0.87905900
C	3.04965700	0.03594500	-0.67923100	C	-3.23840300	-0.66959500	-0.33807700
H	3.00987100	-1.43885600	0.90173200	H	-2.94746700	1.46582600	-0.27985800

H	2.57810200	1.35668900	1.97108500	H	-2.45496100	0.13981700	2.40725400
H	1.79203600	-0.15701800	2.43807000	H	-1.61038800	1.49153900	1.67854400
H	0.83058600	1.83098500	0.55568300	H	-0.89001200	-1.30749600	1.59278400
H	4.22342000	-0.17480100	1.15668100	H	-4.15680100	0.89994000	0.88636700
C	3.87426500	1.28418200	-1.04352500	C	-4.09100800	-1.73266500	0.37917300
H	4.93980500	1.03997100	-1.05169700	H	-5.15113800	-1.47069100	0.31975000
H	3.59191800	1.64466000	-2.03496700	H	-3.94612000	-2.70721000	-0.09207700
H	3.71750800	2.09527900	-0.32636700	H	-3.82026000	-1.82118500	1.43499300
C	3.32214500	-1.10457900	-1.66023500	C	-3.66284300	-0.52679400	-1.79962400
H	3.09176600	-0.79326100	-2.68082400	H	-3.56941900	-1.48276600	-2.31804900
H	4.37587000	-1.39172000	-1.61216800	H	-4.70440100	-0.19851700	-1.85515400
H	2.71265700	-1.97690300	-1.41626100	H	-3.03675100	0.20610600	-2.31289800
N	1.60045600	0.39145400	-0.72307600	N	-1.80529800	-1.07258000	-0.27482600
O	0.97761700	0.63251600	-1.80066800	O	-1.33383300	-2.03223500	-0.95856700
O	-0.93799600	1.69004700	2.70291000	O	0.36777200	3.87534900	0.42652100
H	-0.16064700	2.12144500	3.08057100	H	-0.33284100	4.51242900	0.60456300
H	-1.22927100	2.13714000	1.74748700	H	0.06966700	3.29144400	-0.33257800
				O	0.87980400	2.11813900	2.05259900
				H	1.77870400	2.15302900	2.40732700
				H	0.74251600	1.20397500	1.48969900
IM1-PT12-2W				IM1-PT11-CH			
C	-2.55571900	-0.45866500	-0.63707000	C	2.88127100	-0.43184300	-0.04831500
C	-2.64710800	-1.67235900	-0.07546800	C	3.22203000	0.86092100	0.01981000
C	-1.59421600	-2.16626200	0.82673800	C	2.19483900	1.90757200	0.10397400
C	-0.28642400	-1.33303500	0.92541800	C	0.71099400	1.48083100	0.13924300
C	-0.30775400	0.03218500	0.41735600	C	0.39311300	0.09384000	0.02907000
C	-1.40988100	0.48534300	-0.38639500	C	1.44918300	-0.92015800	-0.03536100
H	-3.50339300	-2.31656700	-0.23372900	H	4.25344700	1.19121400	0.00799600
H	-1.06315800	2.66612900	1.76617900	H	-1.34226800	2.05288000	-0.40930100
Cl	-3.82434900	0.13621200	-1.66682900	Cl	4.09185000	-1.66849600	-0.16198600
O	-1.72757800	-3.18942900	1.46197900	O	2.48692800	3.08243100	0.14297800
O	0.68721600	-1.85548400	1.44511800	O	-0.11463200	2.40206100	0.30488600
O	-1.51718100	1.64851100	-0.83971600	O	1.23516100	-2.12231200	-0.08995400
C	3.27195200	-0.05962500	0.94227200	C	-2.91426700	-1.54280300	0.89980800
C	2.05984600	0.82557200	1.31985600	C	-1.41372300	-1.73299000	0.60647300
C	1.04269700	0.70218500	0.15837000	C	-0.96115500	-0.37520300	0.11642900
C	3.25548700	-0.18218000	-0.59115600	C	-3.35723000	-0.36227100	0.01288600
H	3.14269900	-1.04718000	1.38450000	H	-3.05784700	-1.28368300	1.95148300
H	2.36001200	1.87113000	1.43186700	H	-1.22527000	-2.46521700	-0.18187400
H	1.64344600	0.48636400	2.26892800	H	-0.83874200	-2.06403600	1.46966900
H	0.83973500	1.68741200	-0.27085600	H	-3.49597100	-2.44199500	0.69464800
H	4.21306600	0.36197000	1.30137300	C	-3.90363500	-0.80274400	-1.35311100
C	3.99866800	0.97436600	-1.28516700	H	-4.87709200	-1.28029800	-1.22029000
H	5.07512400	0.88698600	-1.11420300	H	-4.02722600	0.05842500	-2.01171400
H	3.81290300	0.94644700	-2.36101600	H	-3.23336200	-1.51614600	-1.83904900
H	3.67264900	1.94756500	-0.90637900	C	-4.31776800	0.59908300	0.71296400

C	3.75537800	-1.53479100	-1.09785600	H	-4.55348900	1.45236800	0.07578800
H	3.62317600	-1.60788400	-2.17894300	H	-5.24672100	0.07242200	0.94565700
H	4.81776600	-1.65018900	-0.86648900	H	-3.88925300	0.96985200	1.64699100
H	3.20386300	-2.34979600	-0.62494000	N	-2.03757300	0.31005000	-0.20311900
N	1.79700000	-0.05654400	-0.87513200	O	-2.06577600	1.48818100	-0.88011400
O	1.30465200	-0.26226600	-2.02591500				
O	-1.01554900	1.74109500	2.43026200				
H	-0.32376300	1.79734500	3.10305800				
H	-0.77521900	0.94290900	1.74933100				
O	-1.08067500	3.51328300	0.79433200				
H	-1.19596900	2.87462900	-0.00286500				
H	-1.81262100	4.14084300	0.78634000				
IM1-PT11-CH							
C	2.93587800	-0.09230300	-0.02890300				
C	2.86163700	1.24296600	0.06034400				
C	1.56451900	1.94767100	0.13873000				
C	0.30053200	1.07296500	0.08991000				
C	0.45667300	-0.30173400	0.03114800				
C	1.70920100	-0.98963000	-0.05682200				
H	3.74399900	1.87036700	0.08423600				
Cl	4.46682700	-0.90274900	-0.11584000				
O	1.49569700	3.15241400	0.23895800				
O	-0.84154000	1.60389100	0.08345500				
O	1.82248500	-2.20843000	-0.14461200				
C	-2.68111400	-0.32047600	1.51234100				
C	-1.51078600	-1.32524800	1.39461200				
C	-0.83516600	-1.06392100	0.02995200				
C	-3.17741800	-0.08917600	0.08265900				
H	-2.33448100	0.62343400	1.93220400				
H	-1.87534700	-2.35400900	1.43290500				
H	-0.79199900	-1.20194500	2.20274200				
H	-0.70776300	-1.97395000	-0.56187300				
H	-3.48341000	-0.70658400	2.14365000				
C	-4.08185900	-1.23617200	-0.41940500				
H	-5.02678000	-1.18758600	0.12506700				
H	-4.28775100	-1.12339500	-1.48517000				
H	-3.64100800	-2.22061300	-0.24819500				
C	-3.80788800	1.26909900	-0.19380000				
H	-4.02435900	1.38798200	-1.25729100				
H	-4.75021300	1.33354800	0.35545500				
H	-3.14593100	2.07142800	0.12594700				
N	-1.87829600	-0.24386600	-0.71190200				
O	-1.83516600	-0.06651600	-1.89550800				