

Supporting information for: 'Influence of Electronic Effects on One- and Two-Photon Absorption in Porphyrin Isomers

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Optimised Cartesian Coordinates.

P			
C	-1.03798501	2.87010627	0.00000000
C	-0.60781687	4.26469477	0.00000000
C	0.74559521	4.24290349	0.00000000
C	1.13067811	2.83521083	0.00000000
N	0.03312691	2.03105700	0.00000000
H	-1.26432786	5.12312448	0.00000000
H	1.42943929	5.07972287	0.00000000
C	2.45896063	2.39887046	0.00000000
H	3.22775997	3.16299713	0.00000000
C	2.90931822	1.08192303	0.00000000
C	4.26510184	0.61594975	0.00000000
N	2.11324611	-0.03376875	0.00000000
C	4.24263061	-0.75354633	0.00000000
H	5.13101760	1.26038477	0.00000000
C	2.87235808	-1.17491910	0.00000000
H	1.09996005	-0.01700928	0.00000000
C	-2.37959164	2.47662460	0.00000000
H	-3.12337439	3.26513001	0.00000000
C	-2.87235808	1.17491910	0.00000000
C	-4.24263061	0.75354633	0.00000000
N	-2.11324611	0.03376875	0.00000000
C	-4.26510184	-0.61594975	0.00000000
H	-5.08693098	1.42602817	0.00000000
C	-2.90931822	-1.08192303	0.00000000
H	-1.09996005	0.01700928	0.00000000
H	-5.13101760	-1.26038477	0.00000000
H	5.08693098	-1.42602817	0.00000000
C	2.37959164	-2.47662460	0.00000000
H	3.12337439	-3.26513001	0.00000000
C	1.03798501	-2.87010627	0.00000000
C	0.60781687	-4.26469477	0.00000000
N	-0.03312691	-2.03105700	0.00000000
C	-0.74559521	-4.24290349	0.00000000
H	1.26432786	-5.12312448	0.00000000
C	-1.13067811	-2.83521083	0.00000000
H	-1.42943929	-5.07972287	0.00000000
C	-2.45896063	-2.39887046	0.00000000
H	-3.22775997	-3.16299713	0.00000000

Cis-P

C	1.86287400	2.31061700	0.00000000
C	1.97840100	3.74012500	0.00000000
C	0.72367000	4.27422400	0.00000000
C	-0.20748000	3.19128100	0.00000000
N	0.52470500	2.03128300	0.00000000
H	2.92118700	4.26888500	0.00000000
H	0.45063500	5.31982200	0.00000000
C	-1.59466200	3.21499100	0.00000000
H	-2.07950700	4.18483000	0.00000000
C	-2.39008700	2.06810600	0.00000000
C	-3.84454100	2.04137000	0.00000000
N	-1.87906700	0.81422700	0.00000000
C	-4.18780400	0.73590100	0.00000000
H	-4.49135900	2.90837100	0.00000000
C	-2.93994800	-0.02295800	0.00000000
H	-5.17955200	0.30333200	0.00000000
C	2.93550500	1.42713100	0.00000000
H	3.91074900	1.90148000	0.00000000
C	-2.91435400	-1.41644500	0.00000000
H	-3.89164200	-1.89161600	0.00000000
C	2.96826700	0.03762500	0.00000000
C	4.16339300	-0.75441200	0.00000000
N	1.92200000	-0.84201200	0.00000000
C	3.80803000	-2.07137600	0.00000000
H	5.16180800	-0.34022200	0.00000000
C	2.38169700	-2.13439000	0.00000000
H	0.90323000	-0.70858700	0.00000000
H	4.46158300	-2.93203000	0.00000000
C	-1.83391700	-2.29773800	0.00000000
C	-2.00828600	-3.74779300	0.00000000
N	-0.52061000	-1.98061200	0.00000000
C	-0.76961600	-4.28452000	0.00000000
H	-2.96137200	-4.25996200	0.00000000
C	0.15002300	-3.15737800	0.00000000
H	-0.48740100	-5.32875500	0.00000000
C	1.54315400	-3.23991500	0.00000000
H	2.00652800	-4.22020700	0.00000000
H	0.00000000	1.14777900	0.00000000

Pc

C	-0.92950023	2.44004789	0.00000000
C	-1.95039634	3.44298277	0.00000000
C	-3.16760927	2.79742063	0.00000000
C	-2.91797410	1.38446866	0.00000000
N	-1.55937509	1.23026481	0.00000000
H	-1.13032498	0.28037886	0.00000000
H	-1.77432746	4.51016179	0.00000000
H	-4.15079332	3.24966752	0.00000000
C	0.47954976	2.54357905	0.00000000
C	1.29057962	3.74517414	0.00000000
N	1.25929589	1.43787514	0.00000000

C	2.58767767	3.31964529	0.00000000
H	0.92442351	4.76395410	0.00000000
C	2.55192484	1.86404629	0.00000000
H	3.48482760	3.92681039	0.00000000
C	-3.86273798	0.34056655	0.00000000
C	3.70246894	1.04436142	0.00000000
C	-3.70246894	-1.04436142	0.00000000
C	3.86273798	-0.34056655	0.00000000
C	-2.55192484	-1.86404629	0.00000000
C	-2.58767767	-3.31964529	0.00000000
N	-1.25929589	-1.43787514	0.00000000
C	-1.29057962	-3.74517414	0.00000000
H	-3.48482760	-3.92681039	0.00000000
C	-0.47954976	-2.54357905	0.00000000
H	-0.92442351	-4.76395410	0.00000000
C	2.91797410	-1.38446866	0.00000000
C	3.16760927	-2.79742063	0.00000000
N	1.55937509	-1.23026481	0.00000000
C	1.95039634	-3.44298277	0.00000000
H	4.15079332	-3.24966752	0.00000000
C	0.92950023	-2.44004789	0.00000000
H	1.13032498	-0.28037886	0.00000000
H	1.77432746	-4.51016179	0.00000000
H	-4.63547976	-1.60457954	0.00000000
H	-4.89322002	0.68846343	0.00000000
H	4.89322002	-0.68846343	0.00000000
H	4.63547976	1.60457954	0.00000000

Cis-Pc-1

C	2.19986300	-1.31032200	0.00000000
C	3.02513300	-2.46734000	0.00000000
C	2.19454600	-3.56218800	0.00000000
C	0.85138900	-3.08963200	0.00000000
N	0.91016400	-1.72553800	0.00000000
H	0.00000000	-1.17560600	0.00000000
H	4.10546200	-2.46308100	0.00000000
H	2.48339100	-4.60379300	0.00000000
C	2.56063300	0.05655400	0.00000000
C	3.84885900	0.65651800	0.00000000
N	1.64321600	1.05377200	0.00000000
C	3.66589700	2.01863100	0.00000000
H	4.78692700	0.12063500	0.00000000
C	2.26445500	2.26960200	0.00000000
H	4.43098100	2.78220200	0.00000000
C	-0.32487500	-3.86061800	0.00000000
C	1.62021300	3.51983800	0.00000000
C	-1.65859800	-3.49241700	0.00000000
C	0.27796700	3.85572100	0.00000000
C	-2.25649900	-2.21551400	0.00000000
C	-3.69272400	-1.97610900	0.00000000
N	-1.60051100	-1.04074500	0.00000000
C	-3.86156300	-0.63181300	0.00000000
H	-4.45578700	-2.74287400	0.00000000

C	-2.52882500	-0.05672100	0.00000000
H	-4.79080600	-0.07944000	0.00000000
C	-0.87138200	3.03877100	0.00000000
C	-2.23913900	3.53845600	0.00000000
N	-0.87979600	1.69336000	0.00000000
C	-3.04866600	2.45201300	0.00000000
H	-2.52484000	4.58179700	0.00000000
C	-2.17244400	1.29469000	0.00000000
H	-4.12946800	2.42919500	0.00000000
H	-2.36633400	-4.31645900	0.00000000
H	-0.13591600	-4.93055600	0.00000000
H	0.06750000	4.92137200	0.00000000
H	2.31139700	4.35814900	0.00000000
H	0.58053600	1.02379200	0.00000000

Cis-Pc-2

C	-2.65784200	0.67715600	-0.11674600
C	-3.65510100	1.61836500	0.15080300
C	-3.04306400	2.86901100	0.19285800
C	-1.66715300	2.70071800	-0.04185200
N	-1.47779200	1.36190700	-0.24180200
H	-0.65854300	0.88253100	-0.58691900
H	-4.69684500	1.39660600	0.33091900
H	-3.51539500	3.81730600	0.40668200
C	-2.60775800	-0.74731000	-0.13754700
C	-3.69919900	-1.71275900	-0.01198000
N	-1.42535700	-1.33063700	-0.20126400
C	-3.09911900	-2.92096600	0.00458500
H	-4.75451400	-1.48636300	0.05287900
C	-1.65199400	-2.67434200	-0.08892900
H	-3.56367200	-3.89416400	0.09438100
C	-0.67800000	3.73280200	-0.01006900
C	-0.71282300	-3.67889000	-0.01015100
C	0.68477600	3.73160800	0.01019400
C	0.70616000	-3.68016300	0.01023500
C	1.67208100	2.69775500	0.04189800
C	3.04826900	2.86352000	-0.19296500
N	1.48027600	1.35929400	0.24187700
C	3.65800700	1.61174600	-0.15096000
H	3.52231200	3.81094100	-0.40687100
C	2.65905500	0.67237300	0.11671500
H	4.69931900	1.38807000	-0.33120600
C	1.64714000	-2.67730700	0.08899000
C	3.09381100	-2.92653800	-0.00464800
N	1.42294000	-1.33319500	0.20136500
C	3.69607100	-1.71941400	0.01186900
H	3.55660200	-3.90057000	-0.09449500
C	2.60638600	-0.75199800	0.13753700
H	4.75178600	-1.49491900	-0.05308900
H	1.13900200	4.71800000	-0.01665100
H	-1.13048800	4.71999200	0.01682300
H	1.13777600	-4.67739200	-0.03981900
H	-1.14623400	-4.67534100	0.03988200

H 0.66020200 0.88149700 0.58721700

CPC			
C	-2.61474200	0.89392600	0.00000000
C	-4.04293200	0.64774600	0.00000000
C	-4.18391100	-0.70432800	0.00000000
C	-2.84054300	-1.25454100	0.00000000
N	-1.92606000	-0.23606700	0.00000000
H	-4.82234700	1.39696200	0.00000000
H	-5.10357400	-1.27393200	0.00000000
C	-1.08636200	-2.99509700	0.00000000
C	-0.61410900	-4.32292200	0.00000000
N	0.01887800	-2.17401600	0.00000000
C	0.76330000	-4.27452200	0.00000000
H	-1.24440000	-5.20084200	0.00000000
C	1.15795300	-2.91573400	0.00000000
H	-0.07620300	-1.16220600	0.00000000
C	-1.85274400	2.10452800	0.00000000
C	-2.11707100	3.49012200	0.00000000
N	-0.51292800	1.95756900	0.00000000
C	-0.89137500	4.14507700	0.00000000
H	-3.09700700	3.94447800	0.00000000
C	0.12057100	3.15694400	0.00000000
H	0.00000000	1.07792300	0.00000000
H	-0.72539500	5.21300800	0.00000000
H	1.45137900	-5.10771700	0.00000000
C	3.06964600	0.04405500	0.00000000
C	4.24742700	0.90340100	0.00000000
N	1.94789600	0.76077600	0.00000000
C	3.79747300	2.17577800	0.00000000
H	5.27121700	0.55427000	0.00000000
C	2.35258200	2.09116000	0.00000000
H	4.36938400	3.09395400	0.00000000
C	1.52547400	3.19722200	0.00000000
H	2.00053700	4.17288500	0.00000000
C	2.52931600	-2.52282900	0.00000000
H	3.15027100	-3.41537500	0.00000000
C	3.27191600	-1.37795000	0.00000000
H	4.33710500	-1.59600900	0.00000000
C	-2.42962300	-2.56600500	0.00000000
H	-3.17893800	-3.35140500	0.00000000

Cis-CPC-1			
C	0.00000000	0.71163200	2.64379400
C	0.00000000	1.69181900	3.65744500
C	0.00000000	2.93238900	3.03517400
C	0.00000000	2.71051600	1.64111300
N	0.00000000	1.35935400	1.45682400
H	0.00000000	1.49466200	4.71934100
H	0.00000000	3.90020600	3.51591600
C	0.00000000	3.12030900	-0.78594500

C	0.00000000	3.97055300	-1.95625900
N	0.00000000	1.78577900	-1.16170900
C	0.00000000	3.13682800	-3.01926000
H	0.00000000	5.05216100	-1.94762300
C	0.00000000	1.77648000	-2.49019700
C	0.00000000	-0.71163200	2.64379400
C	0.00000000	-1.69181900	3.65744500
N	0.00000000	-1.35935400	1.45682400
C	0.00000000	-2.93238900	3.03517400
H	0.00000000	-1.49466200	4.71934100
C	0.00000000	-2.71051600	1.64111300
H	0.00000000	-1.00629600	0.48711400
H	0.00000000	-3.90020600	3.51591600
H	0.00000000	3.39386800	-4.07006800
C	0.00000000	-1.77648000	-2.49019700
C	0.00000000	-3.13682800	-3.01926000
N	0.00000000	-1.78577900	-1.16170900
C	0.00000000	-3.97055300	-1.95625900
H	0.00000000	-3.39386800	-4.07006800
C	0.00000000	-3.12030900	-0.78594500
H	0.00000000	-5.05216100	-1.94762300
C	0.00000000	-3.56184400	0.52237200
H	0.00000000	-4.63222100	0.69969500
C	0.00000000	0.68261400	-3.42075600
H	0.00000000	1.07630800	-4.43507400
C	0.00000000	-0.68261400	-3.42075600
H	0.00000000	-1.07630800	-4.43507400
C	0.00000000	3.56184400	0.52237200
H	0.00000000	4.63222100	0.69969500
H	0.00000000	1.00629600	0.48711400

Cis-CPc-2

C	-2.07895100	2.12813000	0.00000000
C	-3.49252500	2.41478400	0.00000000
C	-4.10985500	1.19500000	0.00000000
C	-3.05321800	0.19878400	0.00000000
N	-1.86092300	0.81219100	0.00000000
H	-3.95851400	3.39042100	0.00000000
H	-5.17411600	0.99941500	0.00000000
C	-2.07118300	-2.11713500	0.00000000
C	-2.37287000	-3.53554000	0.00000000
N	-0.71000700	-1.91267300	0.00000000
C	-1.18637000	-4.18073300	0.00000000
H	-3.36929000	-3.95733100	0.00000000
C	-0.17149700	-3.14460000	0.00000000
C	-0.85435300	2.86555700	0.00000000
C	-0.35746600	4.19578700	0.00000000
N	0.22234100	2.05262000	0.00000000
C	1.02192200	4.11815200	0.00000000
H	-0.95677200	5.09417600	0.00000000
C	1.39277400	2.73845900	0.00000000
H	0.00000000	1.05865200	0.00000000
H	1.71767900	4.94566800	0.00000000

H	-0.99602000	-5.24561800	0.00000000
C	2.82314500	-1.52242000	0.00000000
C	4.18785300	-1.13367700	0.00000000
N	2.07042600	-0.38454900	0.00000000
C	4.23486100	0.23170400	0.00000000
H	5.01688300	-1.82618400	0.00000000
C	2.90505800	0.73337900	0.00000000
H	5.11248500	0.86283700	0.00000000
C	2.62318800	2.10094400	0.00000000
H	3.50096300	2.73786500	0.00000000
C	1.19882500	-3.52118200	0.00000000
H	1.30875600	-4.60305500	0.00000000
C	2.40641400	-2.87270800	0.00000000
H	3.26452200	-3.53889600	0.00000000
C	-3.12176000	-1.19131000	0.00000000
H	-4.11517000	-1.63314400	0.00000000
H	1.05176100	-0.46617400	0.00000000

Cis-CPc-3

C	0.00000000	0.71812900	2.58300000
C	0.00000000	1.67797200	3.67403100
C	0.00000000	2.90784000	3.09423600
C	0.00000000	2.67668100	1.66085000
N	0.00000000	1.33095100	1.41378400
H	0.00000000	1.44560400	4.73019800
H	0.00000000	3.87190600	3.58500600
C	0.00000000	3.16372200	-0.74996100
C	0.00000000	3.97070300	-1.90493600
N	0.00000000	1.85161700	-1.17055500
C	0.00000000	3.12773200	-2.99565800
H	0.00000000	5.05143200	-1.90681200
C	0.00000000	1.78933600	-2.52837600
C	0.00000000	-0.71812900	2.58300000
C	0.00000000	-1.67797200	3.67403100
N	0.00000000	-1.33095100	1.41378400
C	0.00000000	-2.90784000	3.09423600
H	0.00000000	-1.44560400	4.73019800
C	0.00000000	-2.67668100	1.66085000
H	0.00000000	-3.87190600	3.58500600
H	0.00000000	3.40582600	-4.03995100
C	0.00000000	-1.78933600	-2.52837600
C	0.00000000	-3.12773200	-2.99565800
N	0.00000000	-1.85161700	-1.17055500
C	0.00000000	-3.97070300	-1.90493600
H	0.00000000	-3.40582600	-4.03995100
C	0.00000000	-3.16372200	-0.74996100
H	0.00000000	-5.05143200	-1.90681200
C	0.00000000	-3.56007900	0.60449400
H	0.00000000	-4.62797200	0.79839100
C	0.00000000	0.68378200	-3.43481400
H	0.00000000	1.07642600	-4.44818900
C	0.00000000	-0.68378200	-3.43481400
H	0.00000000	-1.07642600	-4.44818900

C	0.00000000	3.56007900	0.60449400
H	0.00000000	4.62797200	0.79839100
H	0.00000000	-1.13062300	-0.43843200
H	0.00000000	1.13062300	-0.43843200

HPc

C	-2.59723500	-1.72107800	0.00000000
C	-3.99887500	-1.32821100	0.00000000
C	-4.01930000	0.02784100	0.00000000
C	-2.62476000	0.44720700	0.00000000
N	-1.81420200	-0.59241000	0.00000000
H	-4.84493900	-2.00225800	0.00000000
H	-4.88273700	0.67842000	0.00000000
C	-2.05451800	1.74989000	0.00000000
C	-2.61839300	3.03634200	0.00000000
N	-0.69810500	1.89186200	0.00000000
C	-1.57095600	3.94413000	0.00000000
H	-3.67626700	3.25541400	0.00000000
C	-0.36721100	3.20949200	0.00000000
H	0.00000000	1.13888000	0.00000000
C	-2.03177500	-2.97424100	0.00000000
H	-2.66965500	-3.85149600	0.00000000
C	-0.63115900	-3.18134100	0.00000000
C	0.12753900	-4.37651700	0.00000000
N	0.25697200	-2.14750400	0.00000000
C	1.46144100	-4.02066700	0.00000000
H	-0.28509400	-5.37530400	0.00000000
C	1.53243700	-2.60368800	0.00000000
H	-0.08638000	-1.18254300	0.00000000
H	2.31668000	-4.68149900	0.00000000
H	-1.63739700	5.02278700	0.00000000
C	2.60801900	1.72802400	0.00000000
C	4.04317200	1.47377800	0.00000000
N	1.90706100	0.58692200	0.00000000
C	4.19298800	0.13654300	0.00000000
H	4.80816100	2.23825200	0.00000000
C	2.85326700	-0.42768700	0.00000000
H	5.10732000	-0.44158900	0.00000000
C	2.68510400	-1.79597000	0.00000000
H	3.61222200	-2.36176800	0.00000000
C	0.95451400	3.71757800	0.00000000
H	0.99096800	4.80360200	0.00000000
C	2.16809700	3.09323700	0.00000000
H	3.01067400	3.77906300	0.00000000

Cis-HPc 1

C	0.54926500	3.12869900	0.00000000
C	1.80698000	3.79306400	0.00000000
C	2.79185100	2.82793900	0.00000000
C	2.14486800	1.56026100	0.00000000

C	2.63864400	0.23158200	0.00000000
C	3.95831400	-0.25138200	0.00000000
C	3.89097600	-1.63323700	0.00000000
C	2.52908000	-1.99678000	0.00000000
C	-0.77715400	3.56376600	0.00000000
C	-1.85244700	2.67273500	0.00000000
C	-3.26837200	2.96353200	0.00000000
C	-3.90044100	1.75995900	0.00000000
C	-2.86042100	0.74746200	0.00000000
C	-0.56857500	-3.11692800	0.00000000
C	-1.77276700	-3.93592800	0.00000000
C	-2.80952700	-3.07814800	0.00000000
C	-2.24338800	-1.73584700	0.00000000
C	-3.09075700	-0.64647500	0.00000000
C	1.99597800	-3.30770500	0.00000000
C	0.70824300	-3.76165100	0.00000000
H	1.94850800	4.86464400	0.00000000
H	3.86031100	2.98565700	0.00000000
H	4.84656300	0.36342400	0.00000000
H	0.75991500	-0.87898600	0.00000000
H	-0.97473000	4.63034900	0.00000000
H	-3.71285300	3.94965900	0.00000000
H	-4.96519500	1.56844700	0.00000000
H	4.71670800	-2.33026400	0.00000000
H	-1.78986300	-5.01728700	0.00000000
H	-3.86843600	-3.29961600	0.00000000
H	-4.14374500	-0.91697100	0.00000000
H	2.76369300	-4.07656800	0.00000000
H	0.61797800	-4.84426300	0.00000000
H	0.00000000	1.14246000	0.00000000
N	0.82339500	1.78632900	0.00000000
N	1.79758200	-0.84683200	0.00000000
N	-1.65784100	1.32078500	0.00000000
N	-0.86041600	-1.81031000	0.00000000

Cis-HPc 2

C	0.28220900	-3.12995600	0.00000000
C	1.49851300	-3.93420300	0.00000000
C	2.53517700	-3.05985100	0.00000000
C	1.94512200	-1.72450300	0.00000000
C	2.55772900	-0.45107100	0.00000000
C	3.96630700	-0.14184700	0.00000000
C	4.04859100	1.21476000	0.00000000
C	2.68596200	1.70282700	0.00000000
C	-1.05209500	-3.50312000	0.00000000
C	-2.08067800	-2.53944800	0.00000000
C	-3.50039200	-2.66710100	0.00000000
C	-4.02831200	-1.40028300	0.00000000
C	-2.94275500	-0.46878300	0.00000000
C	-0.21881300	3.21143900	0.00000000
C	-1.34908400	4.08554200	0.00000000
C	-2.46941800	3.31655200	0.00000000
C	-2.07639500	1.93897500	0.00000000

C	-3.02614300	0.92330700	0.00000000
C	2.33721600	3.06117400	0.00000000
C	1.10509100	3.68462600	0.00000000
H	1.54461100	-5.01498800	0.00000000
H	3.59178100	-3.28925300	0.00000000
H	4.77529500	-0.85934400	0.00000000
H	-1.32719800	-4.55163200	0.00000000
H	-4.04106400	-3.60286400	0.00000000
H	-5.07370400	-1.12489700	0.00000000
H	4.93815900	1.83054900	0.00000000
H	-1.28201800	5.16397600	0.00000000
H	-3.49935100	3.64518500	0.00000000
H	-4.04403500	1.29973900	0.00000000
H	3.18765300	3.73834800	0.00000000
H	1.14332600	4.76998100	0.00000000
H	0.00000000	1.15141300	0.00000000
H	-0.78749500	-0.95721400	0.00000000
N	0.62245200	-1.81134900	0.00000000
N	1.81024600	0.67254600	0.00000000
N	-1.80344600	-1.20503000	0.00000000
N	-0.69110100	1.92766000	0.00000000

Cis-HPc 3

C	1.56895500	-2.58146800	0.00000000
C	1.29507500	-4.02021600	0.00000000
C	-0.05296800	-4.15659900	0.00000000
C	-0.57878500	-2.79638900	0.00000000
C	-1.90221900	-2.25016300	0.00000000
C	-3.22956500	-2.69520000	0.00000000
C	-4.04052700	-1.56122000	0.00000000
C	-3.20872300	-0.42221400	0.00000000
C	2.78112100	-1.94437700	0.00000000
C	2.99332500	-0.53393500	0.00000000
C	4.32314000	0.06352000	0.00000000
C	4.14183600	1.40472100	0.00000000
C	2.70458900	1.60389200	0.00000000
C	-1.56302700	2.63007800	0.00000000
C	-1.35043500	4.03151700	0.00000000
C	0.00181800	4.27853600	0.00000000
C	0.65832000	3.03366300	0.00000000
C	2.04392600	2.81558800	0.00000000
C	-3.59038700	0.94463900	0.00000000
C	-2.90900000	2.12938500	0.00000000
H	2.03902300	-4.80588400	0.00000000
H	-0.62985500	-5.07106500	0.00000000
H	-3.55231000	-3.72596600	0.00000000
H	-1.05385400	-0.40352000	0.00000000
H	3.67623800	-2.56031800	0.00000000
H	5.25600700	-0.48486400	0.00000000
H	4.89098000	2.18506000	0.00000000
H	-5.12107200	-1.53500200	0.00000000
H	-2.14976600	4.75842600	0.00000000
H	0.49915700	5.23790400	0.00000000

H	2.64925800	3.71716500	0.00000000
H	-4.67025500	1.06318000	0.00000000
H	-3.58232800	2.98148400	0.00000000
H	0.00000000	1.08662700	0.00000000
N	0.38653400	-1.89966600	0.00000000
N	-1.93826900	-0.88887900	0.00000000
N	2.04495500	0.40695800	0.00000000
N	-0.31751300	2.05504900	0.00000000

NCP

C	-1.03418900	2.78752000	-0.06002500
C	-0.59494200	4.17655700	-0.10670200
C	0.75053000	4.15052800	-0.11395500
C	1.13607500	2.74486900	-0.06996100
N	0.03993100	1.94024700	-0.04437600
H	-1.25334700	5.03460200	-0.12624600
H	1.44138100	4.98243900	-0.14045000
C	2.47779100	2.35475600	-0.04018000
H	3.21579000	3.14890700	-0.05967100
C	2.97015000	1.05799000	0.02205100
C	4.30147800	-0.76955200	0.09628700
H	5.19233500	1.23954700	0.07770200
C	2.93595700	-1.20182400	0.07595700
H	1.18268100	0.02886200	-0.09117900
H	5.14853500	-1.43985500	0.13782900
C	-2.38094400	2.44725100	-0.02048900
H	-3.09011500	3.26777700	-0.02460500
C	2.43348900	-2.49208800	0.05500500
H	3.16201800	-3.29268200	-0.03089900
C	-2.92696900	1.16367600	0.03227000
C	-4.28956400	0.75172900	0.09588600
N	-2.17610000	0.02879300	0.01732400
C	-4.31263700	-0.61941200	0.09967700
H	-5.13470400	1.42412800	0.13012000
C	-2.96914200	-1.09262700	0.05125600
H	-1.17777200	0.07686000	-0.13135800
H	-5.18098100	-1.26121300	0.14703400
C	1.07310900	-2.82169600	0.06729100
C	0.49350500	-4.12066300	-0.28741600
H	1.06307300	-5.00844700	-0.54762200
C	-1.17477900	-2.79267300	0.04451200
C	-2.50869000	-2.40811100	0.01362100
H	-3.24867300	-3.19221100	-0.10513400
N	2.18102500	-0.05131900	0.04113800
C	4.32484100	0.59528100	0.06973400
C	-0.03704100	-2.01035000	0.30732800
N	-0.80145200	-4.11408900	-0.30053000
H	-0.03221000	-1.04109300	0.77670300

Trans-N₂CP(1)

C	2.76750300	1.04102200	0.02859700
C	3.32542000	2.33660800	0.43354100
C	1.22859700	2.69735100	0.04383800
H	4.35781300	2.50383500	0.72779900
C	0.06958000	3.46978800	0.00625500
H	0.18958100	4.53991800	0.13259400
C	-1.22859700	2.97169700	-0.10751600
C	-3.48160600	2.72077900	-0.22182400
H	-2.58187400	4.72810200	-0.28550500
C	-2.89083100	1.42591500	-0.11971100
H	-0.88716200	0.93517900	0.24486000
H	-4.54370700	2.90526700	-0.29962400
C	3.47224000	-0.16363500	-0.01451700
H	4.55230400	-0.13311800	0.09133100
C	-3.47224000	0.16363500	-0.01451700
H	-4.55230400	0.13311800	0.09133100
C	2.89083100	-1.42591500	-0.11971100
C	3.48160600	-2.72077900	-0.22182400
N	1.53470000	-1.63508500	-0.08322100
C	2.47676600	-3.65485200	-0.21415400
H	4.54370700	-2.90526700	-0.29962400
C	1.22859700	-2.97169700	-0.10751600
H	0.88716200	-0.93517900	0.24486000
H	2.58187400	-4.72810200	-0.28550500
C	-2.76750300	-1.04102200	0.02859700
C	-3.32542000	-2.33660800	0.43354100
H	-4.35781300	-2.50383500	0.72779900
C	-1.22859700	-2.69735100	0.04383800
C	-0.06958000	-3.46978800	0.00625500
H	-0.18958100	-4.53991800	0.13259400
N	-1.53470000	1.63508500	-0.08322100
C	-2.47676600	3.65485200	-0.21415400
C	-1.41574300	-1.32792300	-0.22850400
N	-2.45218400	-3.29082200	0.44479700
N	2.45218400	3.29082200	0.44479700
C	1.41574300	1.32792300	-0.22850400
H	-0.73291000	-0.70367600	-0.77850300
H	0.73291000	0.70367600	-0.77850300

Trans-N₂CP(2)

C	-2.74576700	1.09211700	-0.16384900
C	-4.06350600	0.52027700	0.13745900
C	-2.74040300	-1.16912200	-0.12939500
H	-4.95508300	1.10014700	0.35930700
C	-2.40377000	-2.52237100	-0.07769600
H	-3.22403200	-3.22705000	0.00014700
C	-1.10650900	-3.03271800	-0.03670400
C	0.73218400	-4.36405600	0.02615400
H	-1.27650300	-5.25069900	-0.10803900
C	1.16294500	-3.00277000	0.09236300
H	-0.00666100	-1.25650600	0.11769000
H	1.39700600	-5.21609500	0.03525500
C	-2.44447800	2.45665300	-0.12856100
H	-3.26865700	3.15927300	-0.05291100

C	2.44447800	-2.45665300	0.12856100
H	3.26865700	-3.15927300	0.05291100
C	-1.16294500	3.00277000	-0.09236300
C	-0.73218400	4.36405600	-0.02615400
N	-0.01662100	2.25488900	-0.05012200
C	0.63681100	4.38231800	0.04098600
H	-1.39700600	5.21609500	-0.03525500
C	1.10650900	3.03271800	0.03670400
H	0.00666100	1.25650600	-0.11769000
H	1.27650300	5.25069900	0.10803900
C	2.74576700	-1.09211700	0.16384900
C	4.06350600	-0.52027700	-0.13745900
H	4.95508300	-1.10014700	-0.35930700
C	2.74040300	1.16912200	0.12939500
C	2.40377000	2.52237100	0.07769600
H	3.22403200	3.22705000	-0.00014700
N	0.01662100	-2.25488900	0.05012200
C	-0.63681100	-4.38231800	-0.04098600
C	1.93427800	0.03785800	0.35743600
N	4.07073700	0.77320600	-0.15769300
N	-4.07073700	-0.77320600	0.15769300
C	-1.93427800	-0.03785800	-0.35743600
H	0.96398100	0.05517700	0.83003700
H	-0.96398100	-0.05517700	-0.83003700

cis-N₂CP(1)

C	-0.81919300	2.93705400	-0.11086600
C	-1.98335000	3.82094500	-0.12349700
C	-2.57097600	1.64933300	-0.09930100
H	-1.94135200	4.90217900	-0.13069800
C	-3.43361500	0.51271900	-0.04714400
H	-4.50134800	0.69775200	-0.06413000
C	-3.02824700	-0.78973800	0.04159700
C	-3.03414800	-3.05843200	0.16584000
H	-4.93114400	-1.97777700	0.09884100
C	-1.65278300	-2.60374100	0.14469600
H	-0.97599000	-0.54862000	-0.01238300
H	-3.31717400	-4.10052200	0.22193200
C	0.46592400	3.38433000	-0.06398800
H	0.60226300	4.46137500	-0.00955800
C	-0.53816400	-3.38743100	0.14276000
H	-0.70499800	-4.45980100	0.12207000
C	1.65037700	2.56922600	-0.03166200
C	2.92841200	2.95089100	0.37030900
H	3.29939500	3.91399600	0.68959400
C	3.00595200	0.74626900	-0.05987300
H	0.93015400	0.61591200	-0.75604000
H	4.69098700	1.84233000	0.65096000
C	0.81156300	-2.91088500	0.08883400
C	2.00182600	-3.67876200	-0.31844000
H	2.00135400	-4.73600400	-0.57151200
C	2.68916500	-1.66516400	-0.01136800
C	3.51830600	-0.59254100	-0.11782900
H	4.57407000	-0.77072200	-0.30487300

N	-1.72661500	-1.22016800	0.08484000
C	-3.85031400	-1.98672600	0.10665000
C	1.28916200	-1.65485000	0.32881400
N	3.08886600	-2.97699200	-0.35871500
H	0.76975400	-0.82228000	0.77004000
C	-3.06948400	3.02764000	-0.12223300
H	-4.11248400	3.31514600	-0.12216800
N	-1.24511700	1.60646800	-0.10530700
N	3.73341400	1.86112000	0.33864800
C	1.73003600	1.19220300	-0.33302100

cis-N₂CP(2)

C	0.81978800	2.93699200	-0.11065500
C	1.98408500	3.82064700	-0.12341000
C	2.57131800	1.64892600	-0.09926500
H	1.94240700	4.90189400	-0.13059000
C	3.43373100	0.51209400	-0.04737400
H	4.50150400	0.69685200	-0.06456600
C	3.02802300	-0.79025300	0.04126100
C	3.03366500	-3.05896800	0.16551000
H	4.93079500	-1.97857900	0.09810600
C	1.65229800	-2.60407500	0.14466300
H	0.97582600	-0.54885400	-0.01207400
H	3.31657800	-4.10108800	0.22165500
C	-0.46526700	3.38433300	-0.06394400
H	-0.60160900	4.46139200	-0.00969200
C	0.53757900	-3.38753200	0.14286000
H	0.70416500	-4.45994000	0.12223800
C	-1.64982900	2.56936300	-0.03160200
C	-2.92792800	2.95150800	0.36973900
H	-3.29867100	3.91474000	0.68890100
C	-3.00592600	0.74681100	-0.05980600
H	-0.92989300	0.61571000	-0.75518100
H	-4.69090900	1.84353600	0.65010200
C	-0.81212600	-2.91075000	0.08916800
C	-2.00254000	-3.67841600	-0.31819100
H	-2.00233100	-4.73562800	-0.57136600
C	-2.68951300	-1.66465100	-0.01117800
C	-3.51843600	-0.59197400	-0.11800500
H	-4.57410300	-0.77013200	-0.30561800
N	1.72639500	-1.22045800	0.08481000
C	3.84996800	-1.98742000	0.10617300
C	-1.28949000	-1.65468300	0.32921400
N	-3.08938100	-2.97640100	-0.35875500
H	-0.76993200	-0.82237900	0.77073500
C	3.07008200	3.02714600	-0.12189000
H	4.11311200	3.31455300	-0.12171800
N	1.24547600	1.60627900	-0.10489200
N	-3.73325400	1.86197400	0.33801800
C	-1.72974700	1.19226300	-0.33246900

NeoCP

C	-3.04582900	-0.05444000	0.01798200
C	-4.22928700	0.80024800	0.00974300
C	-3.77458400	2.06895400	-0.00226200
C	-2.31369700	1.98154900	-0.00178400
N	-1.90147900	0.71827700	0.01184500
H	-5.25469000	0.45496500	0.01219800
H	-4.34955600	2.98522200	-0.01317300
C	-1.44462900	3.10210600	-0.01303400
H	-1.89832900	4.08677700	-0.01589400
C	-0.07363700	3.05850100	-0.01590200
C	0.82666300	4.19588200	-0.00992600
N	0.72295900	1.94280100	-0.01858300
C	2.09561500	3.73404900	-0.00684000
H	0.49540200	5.22484000	-0.00500900
C	2.05424700	2.28508200	-0.01128200
H	0.38219000	0.98938500	-0.04280200
C	-3.09958700	-1.41656600	0.02131900
H	-4.06189300	-1.91396600	0.01361900
C	-2.10920400	-3.66642700	-0.05360200
C	-0.85313900	-4.16912100	-0.06093600
H	-3.07384800	-4.14787300	-0.10146400
C	0.06677900	-3.05295100	0.01277500
H	-0.42092300	-0.88570600	0.14854900
H	-0.58784300	-5.21513100	-0.11868800
H	3.01034600	4.31010800	0.00111000
C	3.12583400	1.43431600	-0.00408700
H	4.10751700	1.89542600	-0.00194500
C	3.07481300	0.01356200	0.00380200
C	4.25586700	-0.84651100	0.00531300
N	1.95076400	-0.69500400	0.00802300
C	3.79279000	-2.11385600	0.00782900
H	5.28276200	-0.50595400	0.00142400
C	2.33788500	-2.02019900	0.01085600
H	4.36018500	-3.03522500	0.00904000
C	1.48761800	-3.09693600	0.00934600
H	1.94926800	-4.08104000	-0.00446300
C	-0.70703800	-1.91245700	0.06979800
N	-2.02159700	-2.26758000	0.02483600

Trans-O₂Pc

C	1.89055983	1.87640881	0.00000000
C	3.21492592	2.35784723	0.00000000
C	4.04270708	1.24699618	0.00000000
C	3.21016107	0.10300965	0.00000000
H	3.50644525	3.39903464	0.00000000
H	5.12444524	1.22986609	0.00000000
C	0.63706911	2.51904218	0.00000000
C	0.39618999	3.96384272	0.00000000
N	-0.51073855	1.81827696	0.00000000
C	-0.95614490	4.09845174	0.00000000
H	1.14493365	4.74638917	0.00000000
C	-1.50335930	2.73389090	0.00000000
H	-1.53282855	5.01605211	0.00000000
C	3.59273240	-1.24665565	0.00000000

C	-2.88383136	2.44647499	0.00000000
C	2.88383136	-2.44647499	0.00000000
C	-3.59273240	1.24665565	0.00000000
C	1.50335930	-2.73389090	0.00000000
C	0.95614490	-4.09845174	0.00000000
N	0.51073855	-1.81827696	0.00000000
C	-0.39618999	-3.96384272	0.00000000
H	1.53282855	-5.01605211	0.00000000
C	-0.63706911	-2.51904218	0.00000000
H	-1.14493365	-4.74638917	0.00000000
C	-3.21016107	-0.10300965	0.00000000
C	-4.04270708	-1.24699618	0.00000000
C	-3.21492592	-2.35784723	0.00000000
H	-5.12444524	-1.22986609	0.00000000
C	-1.89055983	-1.87640881	0.00000000
H	-3.50644525	-3.39903464	0.00000000
H	3.51813035	-3.33137964	0.00000000
H	4.67543254	-1.35603505	0.00000000
H	-4.67543254	1.35603505	0.00000000
H	-3.51813035	3.33137964	0.00000000
O	-1.91633357	-0.51674547	0.00000000
O	1.91633357	0.51674547	0.00000000

cis-O₂Pc (1)

C	0.00000000	0.70716600	-2.55784395
C	0.00000000	1.62484400	-3.61445995
C	0.00000000	2.88866100	-3.03220195
C	0.00000000	2.71313100	-1.63682495
C	0.00000000	-0.70716600	-2.55784395
C	0.00000000	-1.62484400	-3.61445995
C	0.00000000	-2.88866100	-3.03220195
C	0.00000000	-2.71313100	-1.63682495
C	0.00000000	3.72744300	-0.65312495
C	0.00000000	-3.72744300	-0.65312495
C	0.00000000	3.74579200	0.73185105
C	0.00000000	-3.74579200	0.73185105
C	0.00000000	2.68683400	1.67375205
C	0.00000000	2.86493800	3.13982805
N	0.00000000	1.39230600	1.34443005
C	0.00000000	1.61394800	3.66505105
C	0.00000000	0.70148900	2.51206005
C	0.00000000	-2.68683400	1.67375205
C	0.00000000	-2.86493800	3.13982805
C	0.00000000	-1.61394800	3.66505105
C	0.00000000	-0.70148900	2.51206005
O	0.00000000	1.37303200	-1.37493995
O	0.00000000	-1.37303200	-1.37493995
N	0.00000000	-1.39230600	1.34443005
H	0.00000000	1.38253400	-4.66820095
H	0.00000000	3.84419200	-3.53918495
H	0.00000000	-1.38253400	-4.66820095
H	0.00000000	-3.84419200	-3.53918495
H	0.00000000	3.81128900	3.66839105

H	0.00000000	1.32972300	4.71000905
H	0.00000000	-3.81128900	3.66839105
H	0.00000000	-1.32972300	4.71000905
H	0.00000000	4.74317100	1.16783705
H	0.00000000	4.71141000	-1.11886095
H	0.00000000	-4.74317100	1.16783705
H	0.00000000	-4.71141000	-1.11886095

cis-O₂Pc (2)

C	0.00000000	2.58975600	-0.67993600
C	0.00000000	3.64732000	-1.59592400
C	0.00000000	3.07907800	-2.86761600
C	0.00000000	1.68477500	-2.69729700
C	0.00000000	2.53923500	0.73582500
C	0.00000000	3.67331300	1.67294400
C	0.00000000	3.10806200	2.90728400
C	0.00000000	1.64776900	2.69519000
C	0.00000000	0.69122700	-3.69954000
C	0.00000000	0.70465900	3.72957800
C	0.00000000	-0.69122700	-3.69954000
C	0.00000000	-0.70465900	3.72957800
C	0.00000000	-1.68477500	-2.69729700
C	0.00000000	-3.07907800	-2.86761600
C	0.00000000	-3.64732000	-1.59592400
C	0.00000000	-2.58975600	-0.67993600
C	0.00000000	-1.64776900	2.69519000
C	0.00000000	-3.10806200	2.90728400
C	0.00000000	-3.67331300	1.67294400
C	0.00000000	-2.53923500	0.73582500
O	0.00000000	1.40661200	-1.36610500
N	0.00000000	-1.36724000	1.36663800
O	0.00000000	-1.40661200	-1.36610500
N	0.00000000	1.36724000	1.36663800
H	0.00000000	4.69844100	-1.34290000
H	0.00000000	3.59246200	-3.81977100
H	0.00000000	4.72695100	1.42135800
H	0.00000000	3.61139500	3.86715500
H	0.00000000	-3.59246200	-3.81977100
H	0.00000000	-4.69844100	-1.34290000
H	0.00000000	-3.61139500	3.86715500
H	0.00000000	-4.72695100	1.42135800
H	0.00000000	-1.13519500	-4.69255700
H	0.00000000	1.13519500	-4.69255700
H	0.00000000	-1.14507100	4.72604100
H	0.00000000	1.14507100	4.72604100

trans-O₂N7Pc

C	1.91521426	1.86795930	0.00000000
C	3.23909327	2.34767240	0.00000000
C	4.06485252	1.23320792	0.00000000
C	3.22979905	0.09177800	0.00000000

H	3.53364655	3.38810147	0.00000000
H	5.14656276	1.21468092	0.00000000
C	0.65120166	2.49001236	0.00000000
C	0.31444873	3.91391703	0.00000000
N	-0.48936942	1.78421846	0.00000000
H	0.99215067	4.76199921	0.00000000
C	-1.45742409	2.71668972	0.00000000
C	3.59498485	-1.26229581	0.00000000
C	-2.84668789	2.47775968	0.00000000
C	2.86596626	-2.45065927	0.00000000
C	-3.57997417	1.29438921	0.00000000
C	1.48123603	-2.72138459	0.00000000
C	0.92439261	-4.08399959	0.00000000
N	0.49456143	-1.79988937	0.00000000
C	-0.42608397	-3.94131432	0.00000000
H	1.49579393	-5.00482293	0.00000000
C	-0.65836471	-2.49392552	0.00000000
H	-1.17962814	-4.71915668	0.00000000
C	-3.21470589	-0.06153157	0.00000000
C	-4.05655525	-1.19949147	0.00000000
C	-3.23714892	-2.31643358	0.00000000
H	-5.13808977	-1.17412333	0.00000000
C	-1.90827168	-1.84520874	0.00000000
H	-3.53732756	-3.35516515	0.00000000
H	3.48665207	-3.34496605	0.00000000
H	4.67572808	-1.38908968	0.00000000
H	-4.66023740	1.42332327	0.00000000
H	-3.43604164	3.39074219	0.00000000
O	-1.92530293	-0.48568521	0.00000000
O	1.93740595	0.50977546	0.00000000
N	-0.98403054	4.05465774	0.00000000

cis-O₂N7Pc (1)

C	1.39786678	-2.26986984	0.00000000
C	2.56773137	-3.03364746	0.00000000
C	3.62460186	-2.12357402	0.00000000
C	3.07157154	-0.83303373	0.00000000
H	2.62483580	-4.11332349	0.00000000
H	4.68246474	-2.34915259	0.00000000
C	0.03046658	-2.63745611	0.00000000
C	-0.63786807	-3.86081075	0.00000000
H	-0.21068560	-4.85492298	0.00000000
C	-2.11938525	-2.32110896	0.00000000
C	3.76673120	0.39899590	0.00000000
C	-3.38881491	-1.68410129	0.00000000
C	3.39018691	1.72998310	0.00000000
C	-3.79797021	-0.36702507	0.00000000
C	2.10518823	2.33545579	0.00000000
C	1.87094801	3.79665391	0.00000000
N	0.95529587	1.66195740	0.00000000
C	0.52515109	3.95639463	0.00000000
H	2.63508942	4.56535050	0.00000000
C	-0.03438063	2.59562293	0.00000000
H	-0.03721341	4.88159293	0.00000000

C	-3.04730056	0.84305053	0.00000000
C	-3.63188384	2.19983784	0.00000000
C	-2.57986738	3.05700128	0.00000000
H	-4.68875371	2.44021340	0.00000000
C	-1.37971984	2.20953664	0.00000000
H	-2.60264181	4.13952429	0.00000000
H	4.22150928	2.43237166	0.00000000
H	4.84244611	0.23170433	0.00000000
H	-4.87795814	-0.23148549	0.00000000
H	-4.17733531	-2.43134987	0.00000000
O	1.71129248	-0.95038600	0.00000000
O	-0.92428990	-1.67059260	0.00000000
N	-1.71673454	0.89077382	0.00000000
N	-1.96817496	-3.65189204	0.00000000

cis-O₂N₇Pc (2)

C	-1.89143674	-1.91494040	0.00000000
C	-3.20940491	-2.38221491	0.00000000
C	-4.03416750	-1.25821161	0.00000000
C	-3.19709608	-0.13048292	0.00000000
H	-3.51005429	-3.42084980	0.00000000
H	-5.11561149	-1.23519221	0.00000000
C	-0.62461097	-2.54712387	0.00000000
C	-0.26585950	-3.97334900	0.00000000
H	-0.92976282	-4.83254176	0.00000000
C	1.48949696	-2.74192765	0.00000000
C	-3.56431458	1.23160922	0.00000000
C	2.86382405	-2.47648316	0.00000000
C	-2.86406914	2.42418996	0.00000000
C	3.58303750	-1.26620342	0.00000000
C	-1.49770000	2.78031445	0.00000000
C	-0.95207853	4.07588625	0.00000000
C	0.43282542	3.93778574	0.00000000
H	-1.52331419	4.99446546	0.00000000
C	0.70351392	2.56449164	0.00000000
H	1.17411771	4.72481747	0.00000000
C	3.16337700	0.07076873	0.00000000
C	4.07573542	1.23293940	0.00000000
C	3.28691283	2.33727369	0.00000000
H	5.15865541	1.19144100	0.00000000
C	1.90779464	1.82027320	0.00000000
H	3.59337622	3.37616657	0.00000000
H	-3.49722681	3.30870819	0.00000000
H	-4.64555453	1.35025962	0.00000000
H	4.66466245	-1.39271682	0.00000000
H	3.47031572	-3.37894038	0.00000000
O	-1.90295823	-0.54779840	0.00000000
N	1.87380715	0.48978621	0.00000000
O	-0.48084134	1.87714808	0.00000000
N	0.49332429	-1.82999428	0.00000000
N	1.03231346	-4.09236148	0.00000000
