

Electronic Supplementary Materials

for

**Molecular engineering of quinoxaline dyes toward more
efficient sensitizers for dye-sensitized solar cells**

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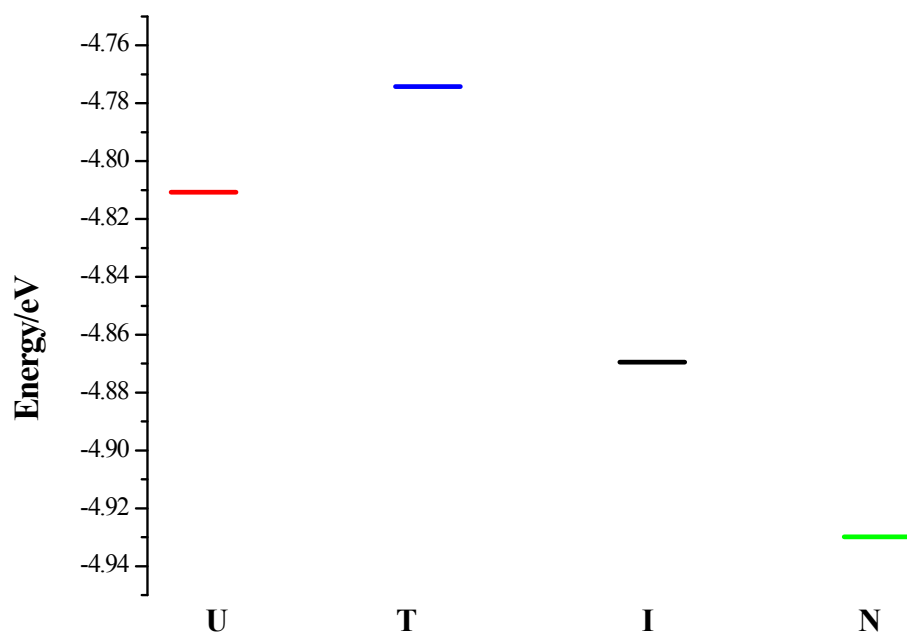


Fig. S1 The energy levels of HOMOs of different donor groups calculated in the CH_2Cl_2 solution. U, T, I and N, represent indoline, triarylamine, ullazine, and N-annulated perylene, respectively.

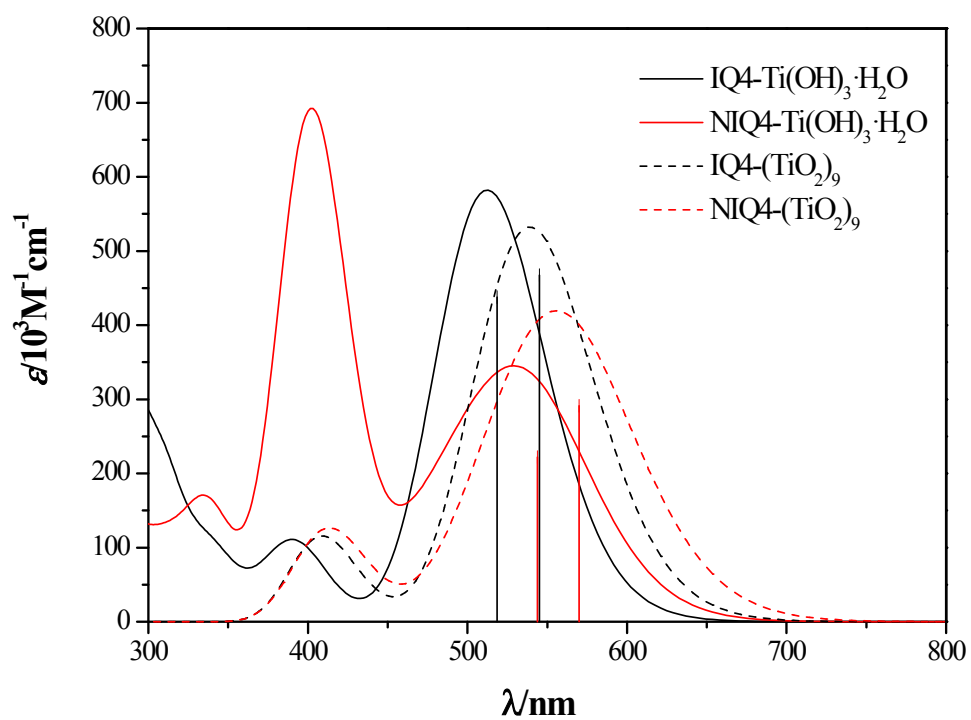


Fig. S2 The absorption spectra of dye-Ti(OH)₃·H₂O (solid line) and dye-(TiO₂)₉ (dash line) complexes.

Table S1 Selected geometry parameters for the neutral and oxidized forms of dyes.

Dye	Bond length (Å) ^a	Torsional angle (°) ^b
UIQ4	1.49	-48.1
UIQ4 ^{•+}	1.49	-47.4
TIQ4	1.48	41.0
TIQ4 ^{•+}	1.48	43.3
IQ4	1.47	42.2
IQ4 ^{•+}	1.47	38.9
NIQ4	1.48	-51.0
NIQ4 ^{•+}	1.48	-49.3

^a Bond length between the carbon atom in benzene ring and the carbon atom in quinoxaline unit.

^b Torsional angle between the donor group and quinoxaline segment.

Table S2 The calculated maximum absorption wavelengths ($\lambda_{\max}^{\text{cal}}$), oscillator strengths (f), transition natures of dye-Ti(OH)₃·H₂O and dye-(TiO₂)₉ complexes (H=HOMO, L=LUMO, etc.).

System	$\lambda_{\max}^{\text{cal}}/\text{nm}(\text{eV})$	f	Assignment
IQ4-Ti(OH) ₃ ·H ₂ O	519(2.39)	1.09	H→L (77%)
IQ4-(TiO ₂) ₉	545(2.27)	1.17	H→L+2 (46%)
NIQ4-Ti(OH) ₃ ·H ₂ O	544(2.28)	0.55	H→L (81%)
NIQ4-(TiO ₂) ₉	570(2.18)	0.73	H→L+1(42%)

Cartesian coordinates of the optimized structures

UIQ4

C	-2.39269300	-0.93249900	-1.22925700
C	-2.82172500	-1.79548500	-2.22914600
C	-4.18056700	-2.03230700	-2.49100100
C	-5.19651500	-1.41489200	-1.76552100
C	-4.79208600	-0.53964100	-0.70348600
C	-3.40811100	-0.29160700	-0.44532300
N	-5.73668900	0.02321900	0.08731300
C	-5.38257400	0.82534800	1.07773000
C	-3.98765000	1.14570900	1.28207500
N	-3.05563500	0.56189300	0.54946200
C	-3.49825400	2.14534100	2.27254400
C	-6.48419300	1.31761900	1.94895800
C	-4.10900200	3.40169200	2.41477400
C	-3.58572200	4.34466900	3.29875400
C	-2.45444500	4.04330600	4.06064300
C	-1.83855000	2.79697800	3.92326300
C	-2.35031800	1.85853300	3.02855600
C	-6.38804200	1.26589500	3.34909800
C	-7.45657700	1.67693600	4.14434200
C	-8.62836100	2.15734700	3.55456800
C	-8.73254900	2.21175200	2.16282600
C	-7.67180200	1.78564000	1.36467000
C	-6.59447100	-1.68988100	-2.10172600
C	-7.03877600	-2.22167600	-3.30972800
C	-8.41629900	-2.46795100	-3.34400800
C	-9.07246400	-2.13671500	-2.16041900
S	-7.93340400	-1.46335000	-0.99783700
C	-10.47306600	-2.31082200	-1.98011700
C	-11.28456900	-2.08676200	-0.89572300
C	-10.80995700	-1.60624600	0.35976000
N	-10.42788900	-1.22204100	1.39128700
H	-2.08315000	-2.29664800	-2.84579100
H	-4.43223900	-2.73275300	-3.27876700
H	-4.98440600	3.64780800	1.82342100
H	-4.06136900	5.31646300	3.39001300
H	-2.05360500	4.77626600	4.75433200
H	-0.95770400	2.55631200	4.51091900
H	-1.86739500	0.89450300	2.90850300
H	-5.48338900	0.89038700	3.81536400
H	-7.37453600	1.61958200	5.22546400

H	-9.45655900	2.48390200	4.17619400
H	-9.64134300	2.58169500	1.69814500
H	-7.75217000	1.81707100	0.28333900
H	-6.38231800	-2.40913600	-4.14955300
H	-8.93773600	-2.87364800	-4.20378300
H	-10.98066100	-2.70016600	-2.85827300
C	-12.74155200	-2.34765700	-0.94081800
O	-13.49491000	-2.17001900	0.00030200
O	-13.16242600	-2.80671000	-2.13952500
H	-14.12136800	-2.94767200	-2.06584600
C	3.79943600	1.00404800	-0.41404100
C	5.16434400	0.72278800	-0.26845100
C	5.33896200	-0.67089200	-0.30831300
C	4.08276100	-1.27178400	-0.46332000
N	3.15826900	-0.22923200	-0.52780100
H	5.94222100	1.46051700	-0.14233000
H	6.27766800	-1.19929500	-0.23849900
C	1.80738000	-0.39388000	-0.68484300
C	0.98345500	0.75726900	-0.69951600
C	1.29943200	-1.70718800	-0.82355000
C	-0.39856800	0.56304900	-0.85722900
C	-0.08945800	-1.84458200	-0.98603300
C	-0.93915200	-0.72541500	-1.00093500
H	-0.50934100	-2.84150200	-1.07571400
C	2.98270900	2.18697200	-0.45041900
C	1.62052600	2.04302900	-0.57944300
C	3.58360500	-2.61477300	-0.58220000
C	2.23253600	-2.80144200	-0.76512000
H	0.99368300	2.92758200	-0.63013700
H	1.83918100	-3.81060900	-0.83522300
C	4.51145900	-3.77061500	-0.51271500
C	5.52283900	-3.85192800	0.45543800
C	4.37713200	-4.84881800	-1.40872000
C	6.37099800	-4.95774500	0.54014300
H	5.63911400	-3.05018300	1.17721400
C	5.21342400	-5.95368000	-1.33839800
H	3.61648300	-4.80765400	-2.18232800
C	6.22033100	-6.01915500	-0.36179400
H	7.13182500	-4.98335900	1.31062400
H	5.11165100	-6.77722800	-2.03774700
C	3.60380600	3.53105500	-0.35289600
C	4.75434000	3.86712600	-1.08097600
C	3.02720700	4.53025400	0.45477700
C	5.31601400	5.14363500	-1.01849600

H	5.21081400	3.12903800	-1.73224000
C	3.57553500	5.80287600	0.52944500
H	2.14663200	4.29672000	1.04544800
C	4.72733500	6.12269200	-0.20745600
H	6.19823400	5.36209600	-1.60743900
H	3.13249500	6.56593400	1.16124300
O	5.18974500	7.39591700	-0.06628300
O	6.98938900	-7.14279200	-0.37638400
C	6.36558900	7.78870100	-0.78727000
C	6.66331900	9.23873900	-0.43591600
H	6.19410900	7.67526700	-1.86634300
H	7.20627700	7.13918500	-0.50803700
C	7.91114100	9.76868000	-1.15310500
H	5.79162600	9.85151800	-0.69688900
H	6.79322100	9.31781100	0.65052100
H	8.77427400	9.13786500	-0.89872000
H	7.77540300	9.67782800	-2.23977200
C	8.23095100	11.22723100	-0.80397300
C	9.47806700	11.76538200	-1.51581400
H	8.36604500	11.31837200	0.28307600
H	7.36798900	11.85913300	-1.05750900
C	9.79409900	13.22173700	-1.16211400
H	10.33941700	11.13209500	-1.26341400
H	9.34180000	11.67400900	-2.60199300
H	10.68875900	13.57522000	-1.68504100
H	8.96505000	13.88444300	-1.43565300
H	9.96887500	13.33884400	-0.08646400
C	8.04191800	-7.27663700	0.58856600
C	8.72874800	-8.61067200	0.33738500
H	7.62282800	-7.23710000	1.60316500
H	8.75101700	-6.44450000	0.48214100
C	9.88426000	-8.87156100	1.31173600
H	7.98269300	-9.41084800	0.41859600
H	9.09911400	-8.62608700	-0.69514700
H	10.62171600	-8.06089200	1.23109000
H	9.50762200	-8.84170600	2.34362400
C	10.58010600	-10.21564700	1.06567900
C	11.73979800	-10.49014200	2.03099500
H	10.95399700	-10.24624300	0.03245200
H	9.84200400	-11.02618200	1.14631100
C	12.42929200	-11.83419000	1.77822800
H	12.47664400	-9.67946500	1.95011500
H	11.36570300	-10.45889900	3.06337500
H	13.25202200	-12.00013300	2.48137600

H	11.72515100	-12.66700600	1.88712100
H	12.84297000	-11.88221800	0.76440100
H	-1.05205300	1.42640000	-0.87400900

TIQ4

N	-3.66550900	-0.52320700	-0.17433600
C	-4.15560500	0.81758900	-0.12819200
C	-5.10511400	1.26090000	-1.05424400
C	-3.71614300	1.71044000	0.86432600
C	-5.61773000	2.55886300	-0.99862100
H	-5.45411100	0.58270500	-1.82624600
C	-4.20502900	3.00854000	0.91450300
H	-2.98725900	1.38040000	1.59737300
C	-5.16462400	3.44521800	-0.01315200
H	-6.35436000	2.86601200	-1.73088500
H	-3.86765700	3.69992600	1.67993600
C	-4.61183300	-1.59029100	-0.25707000
C	-5.69420400	-1.65362700	0.62626300
C	-4.48892000	-2.58424100	-1.24297200
C	-6.64121300	-2.67629900	0.53617300
H	-5.80322500	-0.89192100	1.39160100
C	-5.41386200	-3.61573500	-1.32666400
H	-3.66100700	-2.54470300	-1.94336500
C	-6.50151300	-3.67095800	-0.44006700
H	-7.46823300	-2.69131000	1.23542700
H	-5.32070200	-4.38569100	-2.08573800
C	-2.28686400	-0.78806900	-0.14075700
C	-1.79102100	-1.99323100	0.39655300
C	-1.35389600	0.14099700	-0.64551900
C	-0.42752200	-2.25238300	0.41622100
H	-2.48051900	-2.71951100	0.81120900
C	0.00821500	-0.12190900	-0.60468000
H	-1.70600600	1.06684700	-1.08602000
C	0.51245300	-1.32615100	-0.07611100
H	-0.08099200	-3.18003500	0.86196900
H	0.69387300	0.60457100	-1.02353900
O	-5.58934200	4.73354300	0.13179700
O	-7.35632500	-4.71975100	-0.61279200
C	-8.47842600	-4.85041500	0.26893700
C	-9.24128400	-6.10175200	-0.14010300
H	-9.11779100	-3.96005900	0.19359400
H	-8.12849700	-4.92820400	1.30745900
C	-10.47019400	-6.35837600	0.74077500
H	-9.54664100	-6.00048500	-1.18892300
H	-8.55943500	-6.95975700	-0.09016000
H	-10.15712600	-6.44491900	1.79055800
H	-11.14398100	-5.49164000	0.69248700

C	-11.24027100	-7.62148600	0.33679900
C	-12.47203100	-7.89274600	1.20905800
H	-10.56500100	-8.48758600	0.38386300
H	-11.55188800	-7.53557600	-0.71381000
C	-13.23291000	-9.15767300	0.80045700
H	-12.16019600	-7.97604600	2.25905400
H	-13.14720000	-7.02758000	1.16038100
H	-14.10720600	-9.32235500	1.43864800
H	-13.58454600	-9.09052100	-0.23546200
H	-12.59412200	-10.04516100	0.87516700
C	-6.56494500	5.24507100	-0.78464200
C	-6.87245700	6.67977100	-0.38175200
H	-7.47241400	4.62700900	-0.74584600
H	-6.17072800	5.20211500	-1.80937600
C	-7.89801400	7.34183200	-1.31019400
H	-7.24378200	6.68303900	0.65057300
H	-5.93828900	7.25486800	-0.38456200
H	-7.51318800	7.34110700	-2.33947900
H	-8.81825800	6.74136800	-1.32710400
C	-8.24018100	8.77880100	-0.89830100
C	-9.25510300	9.45521900	-1.82781700
H	-7.31911800	9.37812100	-0.87023700
H	-8.63354800	8.77726200	0.12811800
C	-9.60205100	10.88542100	-1.40350100
H	-8.85754700	9.46318900	-2.85180100
H	-10.17182500	8.85094300	-1.86261200
H	-10.32573900	11.34127600	-2.08711600
H	-10.03635000	10.90518400	-0.39737300
H	-8.70990900	11.52204800	-1.39021200
C	1.95061000	-1.65465600	-0.08033000
C	2.37657800	-2.94705000	-0.37464100
C	3.72996600	-3.30898400	-0.40673300
C	4.75499400	-2.39413200	-0.16570700
C	4.35893400	-1.04852300	0.13201900
C	2.97596300	-0.69259400	0.21677700
N	5.30760000	-0.09768800	0.30815400
C	4.95956300	1.13536800	0.63712600
C	3.57331500	1.44116900	0.91019800
N	2.63515100	0.54559400	0.65404000
C	3.10792400	2.71382200	1.52877400
C	6.05194800	2.14417100	0.67112400
C	3.80028500	3.31232200	2.59425800
C	3.30501200	4.46681700	3.19936500
C	2.11851000	5.04655700	2.74439300

C	1.42063100	4.45617300	1.68795000	
C	1.90609900	3.29385000	1.09148300	
C	5.89463000	3.40580800	0.07415800	
C	6.94955200	4.31677800	0.06274500	
C	8.16982800	3.98686200	0.65766500	
C	8.33487200	2.73436600	1.25341200	
C	7.28668000	1.81516900	1.25239700	
C	6.14719300	-2.83408700	-0.23946900	
C	8.63139800	-3.11636500	-0.56283000	
C	7.95370100	-4.31586800	-0.35223200	
C	6.57498600	-4.15902000	-0.17515000	
H	1.63879500	-3.70077900	-0.62789700	
H	3.97517300	-4.32887300	-0.67922800	
H	4.71928600	2.86729500	2.95984800	
H	3.84570400	4.91152500	4.02934800	
H	1.73855200	5.94974000	3.21239200	
H	0.49632600	4.89962400	1.32985100	
H	1.35877100	2.82511800	0.28098200	
H	4.95160500	3.66805200	-0.39389500	
H	6.81894400	5.28389600	-0.41319500	
H	8.98812800	4.70055900	0.65374400	
H	9.28164100	2.47044400	1.71443000	
H	7.41381300	0.83786600	1.70522100	
H	5.90488100	-4.98762100	0.01347100	
S	7.50704800	-1.76088000	-0.49591400	
H	8.46257700	-5.27306800	-0.32648200	
C	10.03657600	-3.05259200	-0.76835900	
C	10.87232400	-1.99459500	-1.03170800	
H	10.52771900	-4.02040400	-0.71663300	
C	10.42372400	-0.64914100	-1.17251300	
N	10.06556200	0.45245600	-1.29945600	
C	12.33010100	-2.17524400	-1.21212200	
O	13.10512600	-1.26674900	-1.45605400	
O	12.72786700	-3.45972200	-1.07846000	
H		13.68997900	-3.47107700	-1.21616500

IQ4

C	-7.73549200	-2.26079300	1.55458700
C	-7.17085500	-3.10357800	2.71427100
C	-5.64924500	-2.97082200	2.54887100
C	-5.44109900	-3.08238400	1.01671200
C	-6.74321700	-2.48813200	0.38492500
C	-4.33968500	-2.24126800	0.42196000
C	-4.90511800	-1.17143400	-0.30552600
N	-6.29216600	-1.24365800	-0.28390500
C	-2.96903800	-2.38618000	0.51519700
C	-2.10234400	-1.45999300	-0.11219000
C	-2.68539300	-0.41111800	-0.84789800
C	-4.06620700	-0.25743900	-0.96090800
C	-7.20011500	-0.33660500	-0.86178500
C	-8.39612900	-0.79932600	-1.43727300
C	-9.30962200	0.09550300	-1.99133000
C	-9.07232400	1.47596600	-2.00484600
C	-7.88521400	1.92993800	-1.41346000
C	-6.96842200	1.05091500	-0.84208700
C	-10.04731000	2.43702100	-2.64209200
C	-0.64202300	-1.64879600	-0.04019900
C	-0.08780200	-2.92387400	-0.12399100
C	1.29322600	-3.15342800	-0.07778200
C	2.22182100	-2.11826400	0.03999600
C	1.69273700	-0.78844400	0.12780600
C	0.28055700	-0.55928400	0.12977500
N	2.54250300	0.26515500	0.18616300
C	2.07031800	1.49295800	0.32697800
C	0.65277500	1.69920000	0.51881800
N	-0.18865900	0.68992900	0.37322700
C	0.04814500	2.99533200	0.93577200
C	3.06310100	2.59783000	0.24859700
C	0.63929300	3.80095900	1.92285400
C	0.01642000	4.97535300	2.34348900
C	-1.19920100	5.36876000	1.77919700
C	-1.79733400	4.57157100	0.80018800
C	-1.18369400	3.38967700	0.38881800
C	2.81507000	3.74370600	-0.52484800
C	3.77846500	4.74557400	-0.63005100
C	4.99557200	4.62398500	0.04508300
C	5.25076400	3.48738700	0.81567600
C	4.29533500	2.47645500	0.91000700
C	3.64998800	-2.42742600	0.05530700

C	4.19687100	-3.68572100	0.30321500
C	5.58922000	-3.73028400	0.18040700
C	6.16054000	-2.50789000	-0.16977200
S	4.91322300	-1.26994900	-0.30883700
C	7.55974200	-2.33459300	-0.34760700
C	8.30264500	-1.24195300	-0.72545000
C	7.73617500	0.02471500	-1.05080200
N	7.28267100	1.06148600	-1.32920200
H	-8.76361400	-2.52575500	1.29408800
H	-7.72809200	-1.19995100	1.82735300
H	-7.52917000	-2.76773300	3.69216700
H	-7.46883500	-4.15325000	2.59886100
H	-5.08073600	-3.72402300	3.10203800
H	-5.31978600	-1.98445700	2.89688000
H	-5.33440500	-4.13753200	0.74445100
H	-7.16219400	-3.17356100	-0.36086800
H	-2.55364300	-3.20637100	1.09424100
H	-2.04253300	0.28584000	-1.37205100
H	-4.46887400	0.54254000	-1.56939500
H	-8.61412900	-1.86146700	-1.45639300
H	-10.22571900	-0.29370200	-2.42861200
H	-7.67910900	2.99698500	-1.37953300
H	-6.08505400	1.44394900	-0.35256400
H	-11.05976000	2.02358800	-2.66349900
H	-10.07992500	3.38934100	-2.10373700
H	-9.76584900	2.66253600	-3.67851000
H	-0.74407200	-3.77495200	-0.27117600
H	1.64075800	-4.17402600	-0.18831900
H	1.57963700	3.50240600	2.37338100
H	0.48050600	5.58163900	3.11554300
H	-1.67870300	6.28765100	2.10297100
H	-2.74361600	4.86909700	0.35825800
H	-1.65301400	2.76077200	-0.35990600
H	1.87381300	3.84393700	-1.05512700
H	3.57918800	5.62041800	-1.24147400
H	5.74192700	5.40884400	-0.03211600
H	6.19582200	3.38530000	1.34006400
H	4.49275000	1.58863000	1.50089800
H	3.60040000	-4.54428800	0.58297500
H	6.18269900	-4.62303900	0.34336300
H	8.13750200	-3.23513800	-0.15844800
C	9.77626700	-1.30186800	-0.84486000
O	10.47280100	-0.36101900	-1.18469400
O	10.28656700	-2.51485000	-0.53684100

H

11.24988200

-2.44991900

-0.64860500

NIQ4

C	5.49293900	-5.24997500	1.64814200
C	4.09675300	-5.38594000	1.79241700
C	3.23401300	-4.41981200	1.27370400
C	3.87454200	-3.31126700	0.62306800
C	5.27875000	-3.12761000	0.48119000
C	6.08542300	-4.16402400	1.01127700
C	3.06202000	-2.33641800	0.06363400
C	3.45074300	-1.19336500	-0.62055700
C	4.84590400	-0.98826800	-0.76042500
C	5.73527700	-1.92691300	-0.21894800
C	1.73970200	-4.46766200	1.33423500
C	0.97821700	-3.42262900	0.70683700
C	1.67953300	-2.38896800	0.10535100
C	0.98673000	-5.45953700	1.96243200
C	-0.42156300	-5.39166400	1.96628000
C	-1.13234000	-4.37544600	1.33587000
C	-0.44197900	-3.34660700	0.64882000
C	-1.02687900	-2.21566000	-0.07577000
C	-0.24188600	-1.19963500	-0.64528300
C	1.16588800	-1.27586300	-0.54735800
N	2.27085000	-0.51955400	-0.99311400
C	2.20379200	0.74507800	-1.71928000
C	7.19223500	-1.66238300	-0.38323500
C	8.07672500	-1.66148300	0.70577900
C	9.43389300	-1.37903300	0.53760100
C	9.97311800	-1.08266200	-0.72200600
C	9.08116700	-1.07817300	-1.80869500
C	7.72777000	-1.36008100	-1.64742100
C	2.97213700	1.87948500	-1.05685400
C	3.65543100	2.79449700	-1.85387400
C	4.35519000	3.87643500	-1.29006400
C	4.35977800	3.98685200	0.10289200
C	3.68998500	3.07405500	0.94089100
C	2.98561500	2.02894300	0.33750500
C	11.46393100	-0.77216300	-0.94680500
C	11.60925400	0.64751100	-1.54500100
C	12.06035400	-1.80438900	-1.93341600
C	12.27677000	-0.83031100	0.36037400
C	5.09471000	4.86811400	-2.20950500
C	5.77769200	6.00305100	-1.42365200
C	4.08703300	5.50562700	-3.19545700
C	6.18211500	4.11137800	-3.00916000

H	6.13148200	-6.03255800	2.04757700
H	3.70961600	-6.26334800	2.30132700
H	7.16474200	-4.12539100	0.91929300
H	5.24709100	-0.10915500	-1.25212900
H	1.46955100	-6.28987600	2.46830900
H	-0.97459400	-6.16804100	2.48689400
H	-2.21499800	-4.37792600	1.38814500
H	-0.73843800	-0.39797000	-1.17872100
H	1.14346000	1.00364200	-1.80091800
H	2.57207500	0.60214400	-2.74175700
H	7.69899000	-1.86365900	1.70345600
H	10.06956900	-1.38636500	1.41545500
H	9.44720700	-0.85776700	-2.80712100
H	7.07465000	-1.36218200	-2.51537300
H	3.64439600	2.65814800	-2.93191100
H	4.90945200	4.79828600	0.56349100
H	2.45514000	1.30209400	0.94110500
H	11.20291900	1.40295300	-0.86428900
H	11.08659500	0.74103100	-2.50152900
H	12.66601000	0.87950900	-1.71798600
H	11.97719100	-2.82074400	-1.53428300
H	11.55307800	-1.78138300	-2.90245400
H	13.12138700	-1.59358200	-2.10723300
H	12.23721400	-1.82265800	0.82131100
H	11.92299800	-0.09834400	1.09377100
H	13.32713800	-0.60526000	0.14972300
H	6.53758300	5.62371000	-0.73284900
H	5.05562300	6.59201500	-0.84869100
H	6.27756300	6.68174400	-2.12208000
H	3.59698300	4.75420100	-3.82145200
H	3.30756900	6.05579600	-2.65795800
H	4.60120500	6.20845200	-3.86034700
H	5.75424500	3.31227800	-3.62150800
H	6.91976600	3.66092900	-2.33665300
H	6.70906100	4.80016900	-3.67873900
C	-2.49326000	-2.17462200	-0.30497400
C	-3.16007300	-3.29035100	-0.80096000
C	-4.53891500	-3.29805100	-1.05301600
C	-5.34150400	-2.17561900	-0.85585700
C	-4.69017100	-0.99829800	-0.35681200
C	-3.28955800	-1.00462800	-0.06125000
N	-5.40192100	0.14577600	-0.21338400
C	-4.81626200	1.23910700	0.24610200
C	-3.44463500	1.18149300	0.69998400

N	-2.72377500	0.09131300	0.50654900
C	-2.76934400	2.29227000	1.42619000
C	-5.62089800	2.49038600	0.20668100
C	-3.40763600	2.98764100	2.46570800
C	-2.73382200	3.99064700	3.16160300
C	-1.42130900	4.32453900	2.81938100
C	-0.77845300	3.63652100	1.78724400
C	-1.44273600	2.61865400	1.10485800
C	-6.97306100	2.46785600	0.58220300
C	-7.75220500	3.62033900	0.49265100
C	-7.19607600	4.80774900	0.01126700
C	-5.85501700	4.83621100	-0.37957600
C	-5.07010600	3.68870900	-0.27802400
C	-6.76818600	-2.24492000	-1.17170500
C	-7.38195600	-3.24274900	-1.92752300
C	-8.77218500	-3.11226800	-2.01158000
C	-9.27417100	-2.01284800	-1.31704400
S	-7.95692900	-1.10613700	-0.58090900
C	-10.65872700	-1.69302000	-1.26859200
C	-11.33876900	-0.69308100	-0.61687900
C	-10.70952500	0.27678400	0.21677700
N	-10.20510500	1.06552500	0.91060800
H	-2.59586700	-4.19178800	-1.01179700
H	-4.98105100	-4.21908000	-1.41371900
H	-4.42736200	2.73637600	2.73774400
H	-3.23528000	4.51203900	3.97129800
H	-0.90266400	5.11437700	3.35441700
H	0.23944000	3.89150900	1.50908400
H	-0.94201400	2.07398200	0.31159100
H	-7.41363100	1.54726600	0.94717000
H	-8.79448800	3.57898700	0.79188600
H	-7.80401100	5.70452100	-0.06316300
H	-5.41901900	5.75200100	-0.76732500
H	-4.03188500	3.71920700	-0.59098300
H	-6.83418600	-4.03693200	-2.41762800
H	-9.41123400	-3.79221300	-2.56378700
H	-11.28376800	-2.37048200	-1.84377700
C	-12.80928500	-0.55253800	-0.71553600
O	-13.45027600	0.31509300	-0.14859400
O	-13.38093300	-1.48848800	-1.50415900
H	-14.33694300	-1.31289900	-1.50108700
C	3.79435100	3.23347600	2.47099700
C	5.27416200	3.05635900	2.89077400
H	5.92098500	3.80252500	2.41976600

H	5.37638100	3.16118800	3.97666800	
H	5.64385400	2.06482600	2.60905200	
C	3.31283200	4.64068400	2.89553600	
H	2.26055300	4.79385300	2.63433600	
H	3.41108600	4.76030600	3.98008900	
H	3.89477100	5.43572500	2.42091300	
C	2.95245500	2.18962800	3.22920900	
H	1.88855000	2.26469100	2.98218600	
H	3.28173200	1.16729600	3.01772700	
H		3.05413400	2.35086700	4.30719600

IQ4-Ti(OH)₃·H₂O

C	-9.30377400	-2.60954700	1.40520400
C	-8.70235000	-3.48356300	2.52197800
C	-7.18898200	-3.28128600	2.35368600
C	-6.99116300	-3.33677300	0.81866600
C	-8.31396500	-2.75504000	0.22160300
C	-5.91993400	-2.44050400	0.25496700
C	-6.52219700	-1.35394400	-0.41568200
N	-7.90383100	-1.46679400	-0.38553200
C	-4.54607700	-2.54250300	0.34563500
C	-3.71426300	-1.55647800	-0.23666800
C	-4.33333600	-0.49831800	-0.93138400
C	-5.71794800	-0.38557500	-1.03606000
C	-8.84613400	-0.52603100	-0.83439400
C	-10.06908700	-0.95710200	-1.37719400
C	-11.02261300	-0.03146700	-1.79709300
C	-10.79875800	1.34851100	-1.70366900
C	-9.58372200	1.76892800	-1.14443400
C	-8.62657800	0.85767000	-0.70494300
C	-11.81740700	2.34659800	-2.19999100
C	-2.25045800	-1.67327500	-0.14879500
C	-1.61687400	-2.91101900	-0.24777000
C	-0.22519800	-3.05461800	-0.17623700
C	0.63617500	-1.96399300	-0.02862600
C	0.02288900	-0.67127700	0.05525400
C	-1.39991700	-0.53354900	0.05542900
N	0.80006500	0.43586000	0.10470700
C	0.25036900	1.63072900	0.24590200
C	-1.17400800	1.73833300	0.47198500
N	-1.94648100	0.67653100	0.32635900
C	-1.85749100	2.98114400	0.91900500
C	1.15902500	2.79783900	0.12576200
C	-1.27687000	3.84315600	1.86391300
C	-1.96515700	4.97232600	2.30566800
C	-3.23786300	5.26125000	1.80553800
C	-3.82618800	4.40465800	0.87060800
C	-3.14523300	3.26820600	0.43685400
C	0.77081500	3.94964100	-0.57969400
C	1.65420100	5.01760700	-0.72418600
C	2.93252200	4.95314700	-0.16137000
C	3.32823400	3.80842300	0.53490700
C	2.45038000	2.73427300	0.67226100
C	2.07968800	-2.17259000	0.02771400

C	2.70602700	-3.40367800	0.23381200
C	4.10096600	-3.34003100	0.19988300
C	4.59684200	-2.05653900	-0.03500300
S	3.27016900	-0.90392300	-0.18700900
C	5.98229100	-1.76922700	-0.10827200
C	6.66119800	-0.59886900	-0.36029000
C	6.03711700	0.65127000	-0.63236200
N	5.54632300	1.68184300	-0.86749600
H	-10.32582000	-2.89061700	1.13853700
H	-9.32309800	-1.56137000	1.72286100
H	-9.06801800	-3.20905900	3.51611200
H	-8.95782000	-4.53771700	2.35546100
H	-6.58179000	-4.02348700	2.87974900
H	-6.90124200	-2.29021200	2.72525400
H	-6.85604400	-4.37749400	0.50760800
H	-8.71713700	-3.41335800	-0.55645800
H	-4.10422400	-3.37054000	0.89303400
H	-3.71428700	0.24052300	-1.42576900
H	-6.15201600	0.42429000	-1.60920900
H	-10.27652100	-2.01750100	-1.47093300
H	-11.96007400	-0.39378300	-2.21187300
H	-9.38822600	2.83244700	-1.02969500
H	-7.72039300	1.21784600	-0.23189900
H	-12.82791700	1.92725800	-2.18833900
H	-11.81816900	3.25481000	-1.58887300
H	-11.60288100	2.65190700	-3.23202300
H	-2.21638900	-3.79863800	-0.42104600
H	0.18443500	-4.05171100	-0.28847200
H	-0.29035000	3.62501100	2.25836700
H	-1.50790600	5.62546100	3.04294900
H	-3.76897700	6.14552900	2.14527800
H	-4.81641500	4.62103500	0.48043900
H	-3.60361300	2.59117000	-0.27629400
H	-0.21873300	4.00335500	-1.02084300
H	1.34619500	5.89869200	-1.27921200
H	3.61812300	5.78822900	-0.27118400
H	4.32568900	3.74165300	0.95621300
H	2.75718100	1.83860300	1.20092500
H	2.16178500	-4.31956700	0.42290800
H	4.75049200	-4.19614800	0.34577100
H	6.62808500	-2.62943800	0.05535100
C	8.12857800	-0.60424700	-0.37839600
O	8.79679600	0.44928100	-0.63235200
O	8.79341200	-1.67959800	-0.13844400

Ti	10.59947100	-0.72144700	-0.39815800	
O	10.79816900	-1.31121500	-2.10230300	
H	11.25124400	-0.77918200	-2.77157500	
O	11.66676600	-1.88481600	0.53775900	
O	11.49565500	0.86910800	-0.44185400	
O	10.12855000	-0.12368700	1.81833900	
H	12.05347000	-2.63696900	0.06719400	
H	11.00112100	1.66809200	-0.67788500	
H	10.63168700	-0.77043600	2.33674300	
H		10.56756500	0.72528600	1.97472500

NIQ4-Ti(OH)₃·H₂O

C	7.01237000	-4.20553400	2.04013800
C	5.66518700	-4.62218400	1.99312200
C	4.80259100	-4.13274000	1.01160900
C	5.38999200	-3.22262300	0.06805600
C	6.71010900	-2.69587600	0.16112300
C	7.53216500	-3.25356200	1.17033500
C	4.56952200	-2.68239500	-0.91716200
C	4.87679400	-1.63047900	-1.76779700
C	6.18483800	-1.09888300	-1.69086800
C	7.06976000	-1.60367100	-0.73392900
C	3.32837700	-4.37856000	0.96577200
C	2.53212100	-3.68206000	-0.00812800
C	3.19083300	-2.88202800	-0.93460200
C	2.61652700	-5.14220200	1.89028500
C	1.20589000	-5.16202100	1.87056200
C	0.45618900	-4.41119500	0.97286500
C	1.10811600	-3.62473300	-0.00932700
C	0.47487700	-2.69162900	-0.93282200
C	1.20913300	-1.85633900	-1.78392600
C	2.61677000	-1.94266800	-1.78319300
N	3.66642600	-1.17749200	-2.35226100
C	3.49429900	0.26399100	-2.63087100
C	8.34301700	-0.85872400	-0.54072300
C	8.63998600	-0.27571900	0.70035000
C	9.76854900	0.52737200	0.86939600
C	10.65007800	0.78521800	-0.19035600
C	10.35006200	0.19103600	-1.42886400
C	9.22340600	-0.60917000	-1.60486000
C	3.96439100	1.06010400	-1.41881000
C	4.94093200	2.04267100	-1.53687600
C	5.58092600	2.57228900	-0.39905700
C	5.18926300	2.08968100	0.85248300
C	4.18087200	1.11840200	1.00497000
C	3.56861300	0.63194500	-0.14442800
C	11.88823700	1.68475100	-0.04785300
C	11.76026000	2.88408000	-1.01657900
C	13.15707000	0.87320600	-0.39858200
C	12.04679800	2.23822200	1.38031000
C	6.71359100	3.59728500	-0.58019000
C	7.41334400	3.94065300	0.74814300
C	6.12596100	4.89391000	-1.18254200
C	7.78423300	3.01985200	-1.53631600

H	7.65641500	-4.62135600	2.80963500
H	5.30870700	-5.31256500	2.75117500
H	8.56194100	-2.93048400	1.27686300
H	6.48000900	-0.23024000	-2.26706600
H	3.13322900	-5.70415900	2.66195200
H	0.68674000	-5.75866400	2.61513000
H	-0.62530100	-4.41492600	1.04799300
H	0.67746200	-1.13950800	-2.39907400
H	2.43957800	0.42861400	-2.86666700
H	4.07101600	0.53599300	-3.51915500
H	7.96277600	-0.42854600	1.53511900
H	9.94107600	0.96484300	1.84562400
H	11.00250100	0.35998400	-2.28025100
H	9.01655900	-1.04523900	-2.57822200
H	5.25678100	2.35148700	-2.52924300
H	5.69446200	2.45066400	1.73943000
H	2.81123200	-0.13562000	-0.06988600
H	10.87298700	3.47956900	-0.77863300
H	11.67733700	2.55905500	-2.05795300
H	12.63996600	3.53259800	-0.93706200
H	13.26986000	0.01744500	0.27544800
H	13.12573200	0.49302100	-1.42398600
H	14.04848000	1.50316100	-0.30311700
H	12.16277000	1.43570700	2.11614900
H	11.18891600	2.85260800	1.67329100
H	12.93989500	2.86891100	1.43319300
H	7.86041200	3.05080900	1.20404700
H	6.72589200	4.39380000	1.46983700
H	8.21863600	4.65899800	0.56251500
H	5.64473500	4.70452500	-2.14724400
H	5.37686000	5.32969900	-0.51242900
H	6.91685300	5.63584400	-1.34079800
H	7.37969400	2.80826400	-2.53023600
H	8.20483600	2.09321100	-1.13675500
H	8.60178100	3.73824000	-1.66230700
C	-1.00117200	-2.55498100	-0.93860500
C	-1.83107400	-3.64230300	-1.17787200
C	-3.23053500	-3.53035700	-1.18349400
C	-3.88057600	-2.31487800	-0.97059200
C	-3.05222200	-1.17235300	-0.71036100
C	-1.62932800	-1.29442800	-0.67427500
N	-3.62706800	0.04095000	-0.53386700
C	-2.87747000	1.09968900	-0.27923300
C	-1.45057000	0.94255100	-0.09393200

N	-0.87141000	-0.22165800	-0.32404900
C	-0.56473900	2.03644000	0.38730800
C	-3.57340600	2.41153500	-0.24554200
C	-0.92730100	2.84400600	1.47801900
C	-0.06227700	3.83718700	1.93438900
C	1.16785800	4.04506200	1.30118600
C	1.53782900	3.24270400	0.21954400
C	0.67869700	2.23949100	-0.22846200
C	-4.84020300	2.51302600	0.35107200
C	-5.52849500	3.72536700	0.34668300
C	-4.96621500	4.84853300	-0.26606300
C	-3.71208400	4.75246600	-0.87635500
C	-3.01679600	3.54442800	-0.86335200
C	-5.34070600	-2.24869100	-1.02378200
C	-6.17753500	-3.22945100	-1.55740500
C	-7.53952500	-2.94414800	-1.41754300
C	-7.79149000	-1.73753000	-0.76343800
S	-6.27975400	-0.93076600	-0.36168000
C	-9.09859100	-1.25054200	-0.50571100
C	-9.53455600	-0.13060500	0.16267300
C	-8.67275800	0.81292400	0.79075700
N	-7.97505800	1.58186700	1.31975400
H	-1.38498600	-4.61292100	-1.36840600
H	-3.80960100	-4.43004400	-1.35555800
H	-1.88284600	2.68937100	1.96836400
H	-0.34739200	4.44885100	2.78515000
H	1.83794700	4.82261300	1.65592000
H	2.50054300	3.37810500	-0.26283200
H	0.96788200	1.60221200	-1.05624700
H	-5.28411800	1.64312000	0.82086400
H	-6.50522400	3.77814400	0.81606800
H	-5.50310800	5.79272400	-0.27229300
H	-3.27507600	5.61806700	-1.36536200
H	-2.04555400	3.47640600	-1.34148300
H	-5.80783100	-4.11965400	-2.04914200
H	-8.33466000	-3.58680300	-1.77903000
H	-9.89841300	-1.87777500	-0.89350900
C	-10.97632300	0.12700000	0.27918100
O	-11.42403800	1.13599500	0.91206400
O	-11.83547800	-0.66477300	-0.25708800
C	3.84830000	0.55414800	2.39528900
C	5.08756500	-0.21555200	2.91399400
H	5.96099200	0.43927400	2.99724300
H	4.88828600	-0.63870500	3.90517100

H	5.34425400	-1.03695600	2.23614000
C	3.49897100	1.70347900	3.36657100
H	2.62513100	2.25781800	3.01007800
H	3.27158100	1.30236800	4.36049000
H	4.32603400	2.41137500	3.47666700
C	2.65709300	-0.42456900	2.35624100
H	1.75307500	0.05305100	1.96355600
H	2.87190900	-1.30635800	1.74376300
H	2.43818500	-0.77548400	3.36990400
Ti	-13.42399100	0.46081500	0.42820400
O	-13.72171500	-0.62910900	1.84773500
H	-14.06976700	-0.28543000	2.68264200
O	-14.69222400	-0.10571500	-0.77040700
O	-14.00386000	2.07086000	1.06257400
O	-12.84622600	1.67594700	-1.48725300
H	-15.20951100	-0.89579900	-0.55839600
H	-13.37357700	2.64793400	1.51897300
H	-13.48191400	1.36429100	-2.14980900
H	-13.07960000	2.60152700	-1.32436700