Supporting Information

Metal-Free Catalysts for Hydrogenation of both Small and Large Imines: A Computational Experiment

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Contents:

SI1 The optimized structures for **im2/cat1** hydrogenation

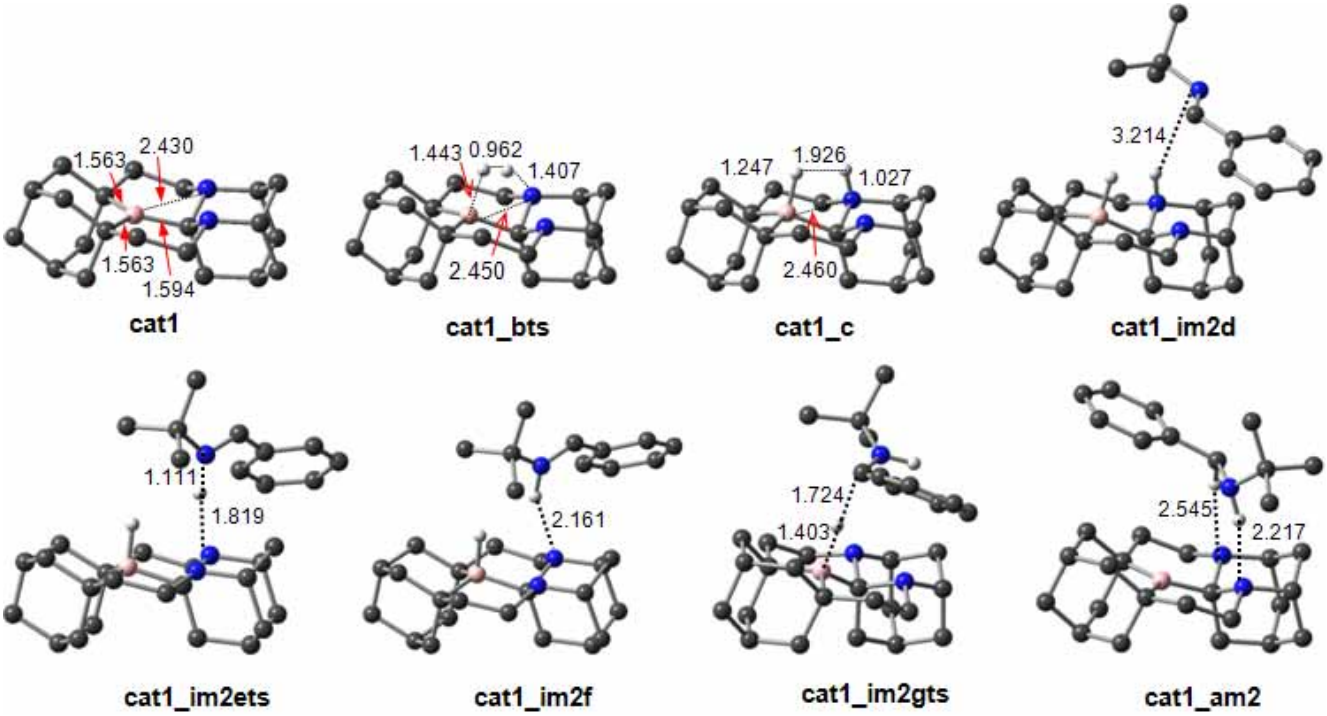

Fig. S1 Optimized structures of the stationary points along the reaction pathway for **im2**/**cat1** hydrogenation, along with the key bond distances in Å. Trivial hydrogen atoms are omitted for clarity.

SI2 The optimized structures for **im1/cat2** hydrogenation

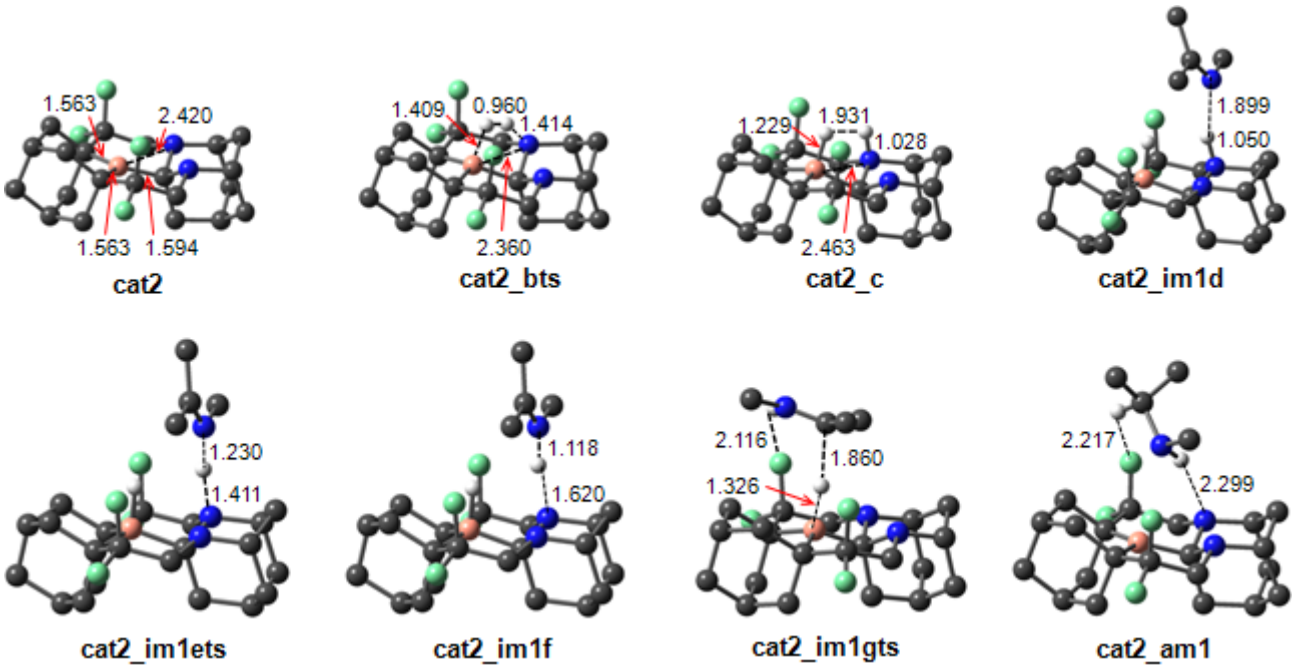

Fig. S2 Optimized structures of the stationary points along the reaction pathway for **im1**/**cat2** hydrogenation, along with the key bond distances in Å. Trivial hydrogen atoms are omitted for clarity.

SI3 The optimized structures and energetics of various complexes for **im2/(cat3** or **cat4)** hydrogenation s

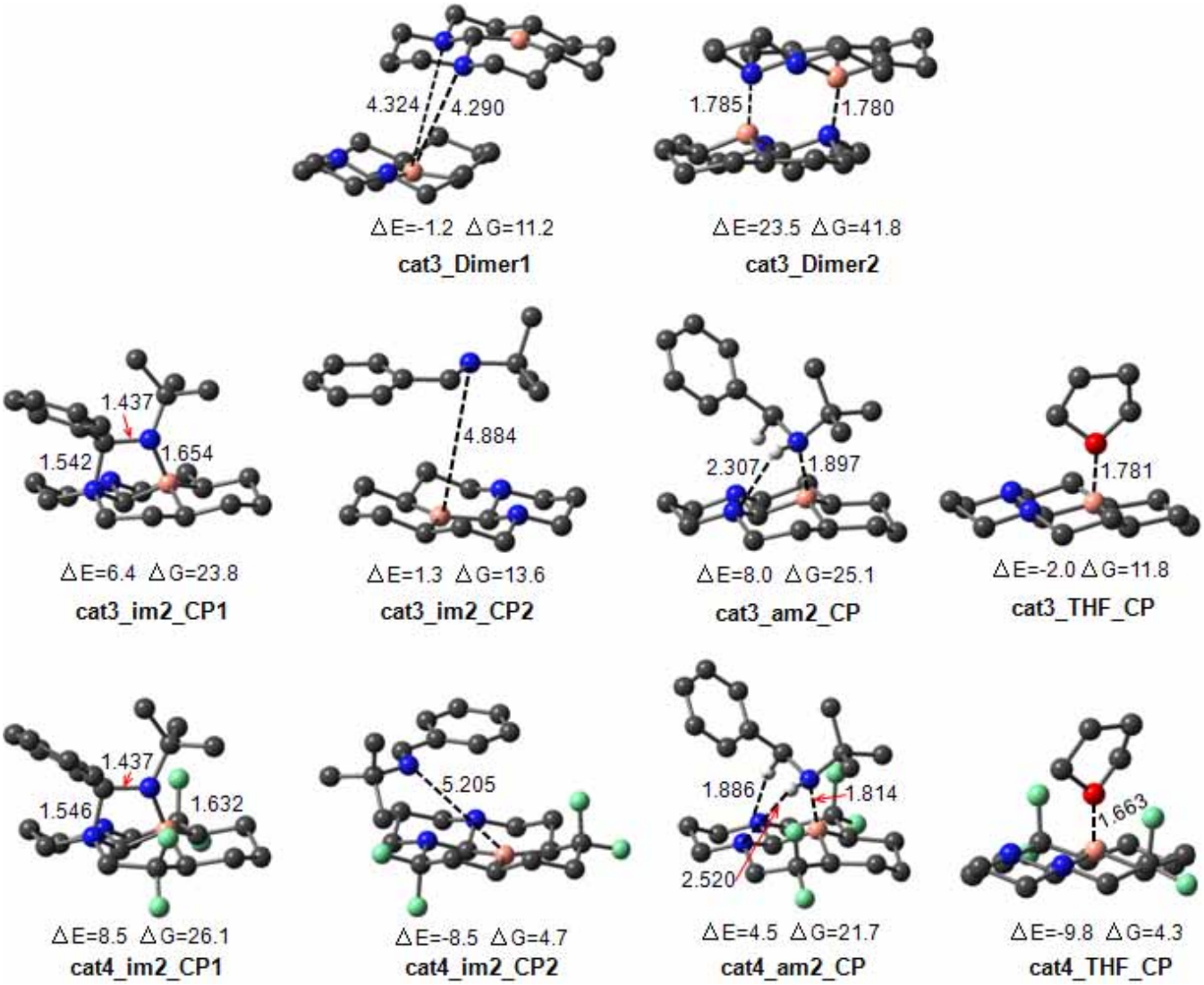

Fig. S3 Optimized structures and energetics of various complexes between **cat3**/**cat4**, **im2** (*t*BuN=C(H)Ph), **am2** (*t*BuNH-CH_2Ph) or THF. The ΔE and ΔG values are the binding energies and free Gibbs free energies (kcal/mol) at the M05-2X/6-311++G(2d,p)(IEFPCM)/M05-2X/6-31G(d,p) + ZPE level.

SI4 The optimized structures for **im2/cat3** hydrogenation

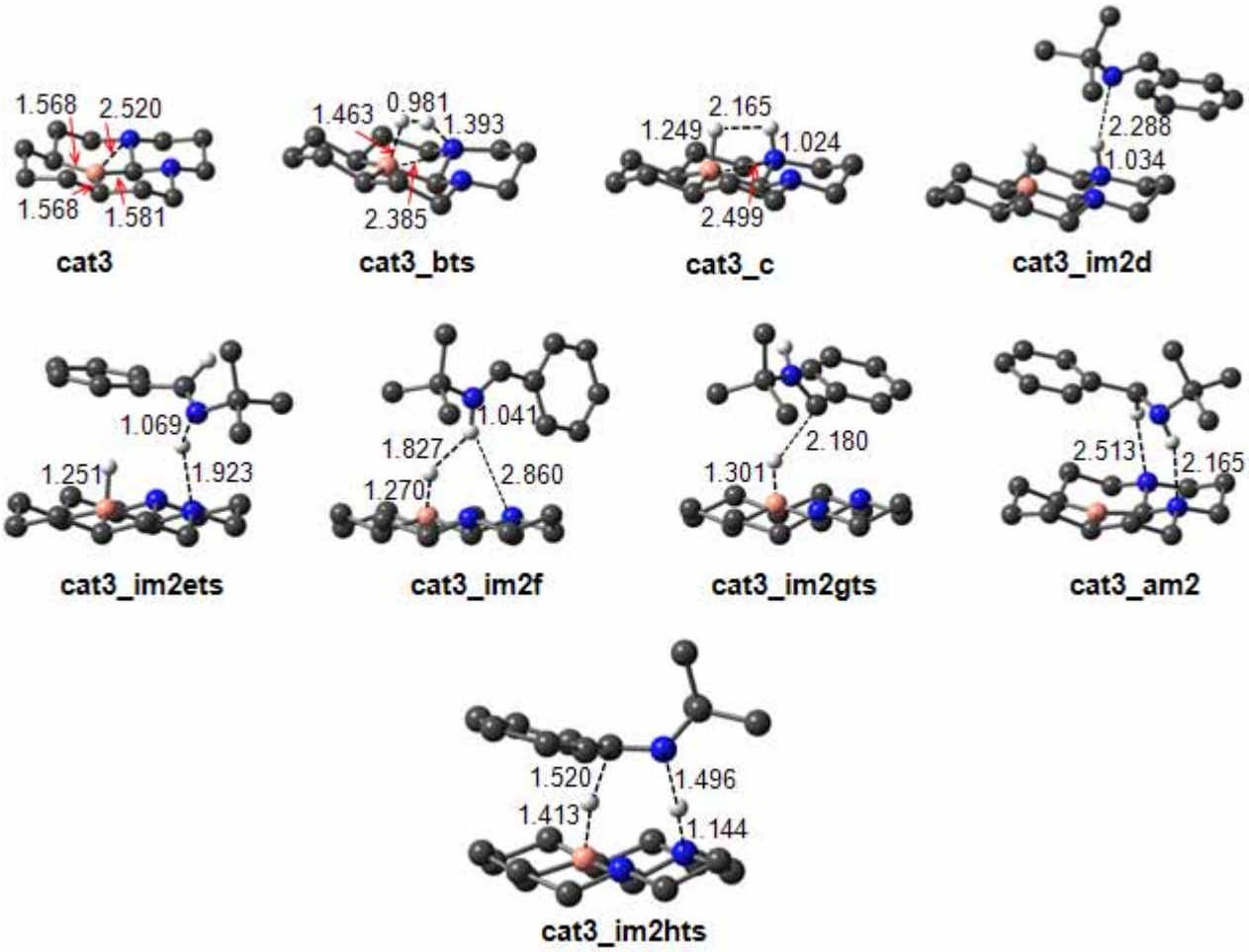

Fig. S4 Optimized structures of the stationary points along the reaction pathway for **im2**/**cat3** hydrogenation, along with the key bond distances in Å. Trivial hydrogen atoms are omitted for clarity.

SI5 The details on the two experimental hydrogen activation systems

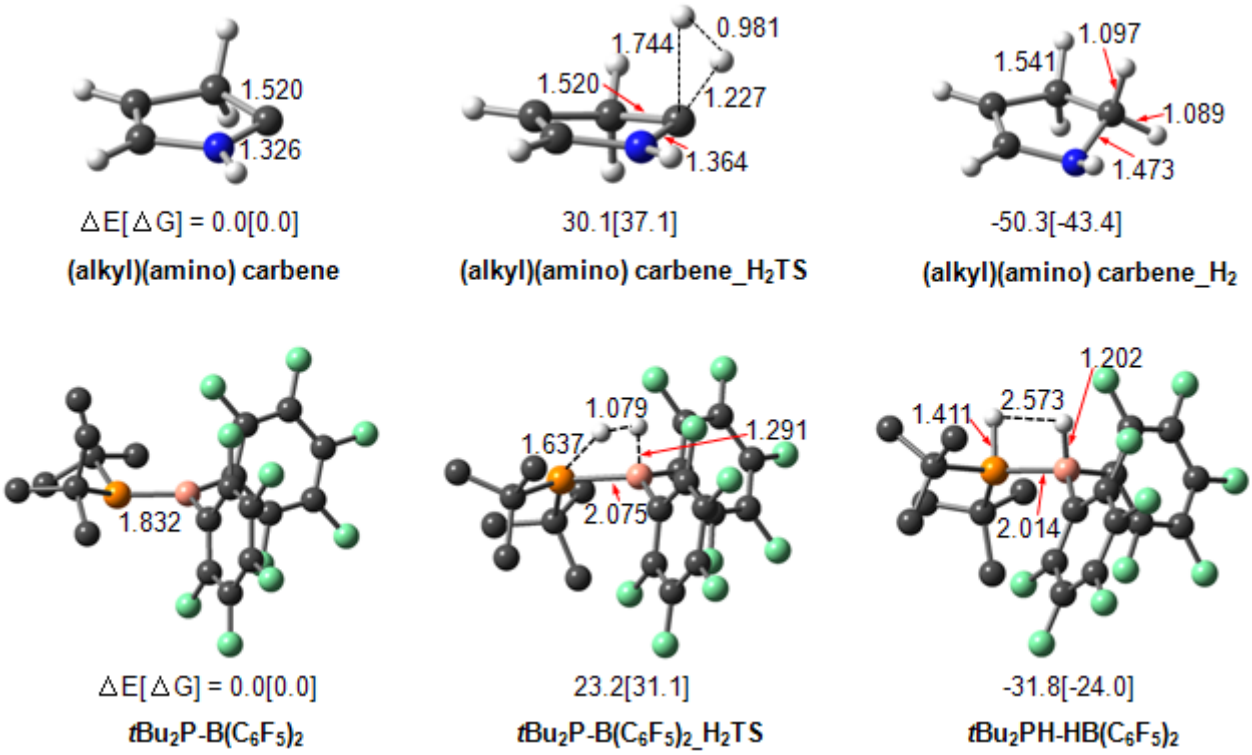

Fig. SI5 The energetic and geometric results about the two experimental hydrogen activation systems.

SI6 The optimized structures and energetics of various complexes for **im1/(cat3** or **cat4)** hydrogenations

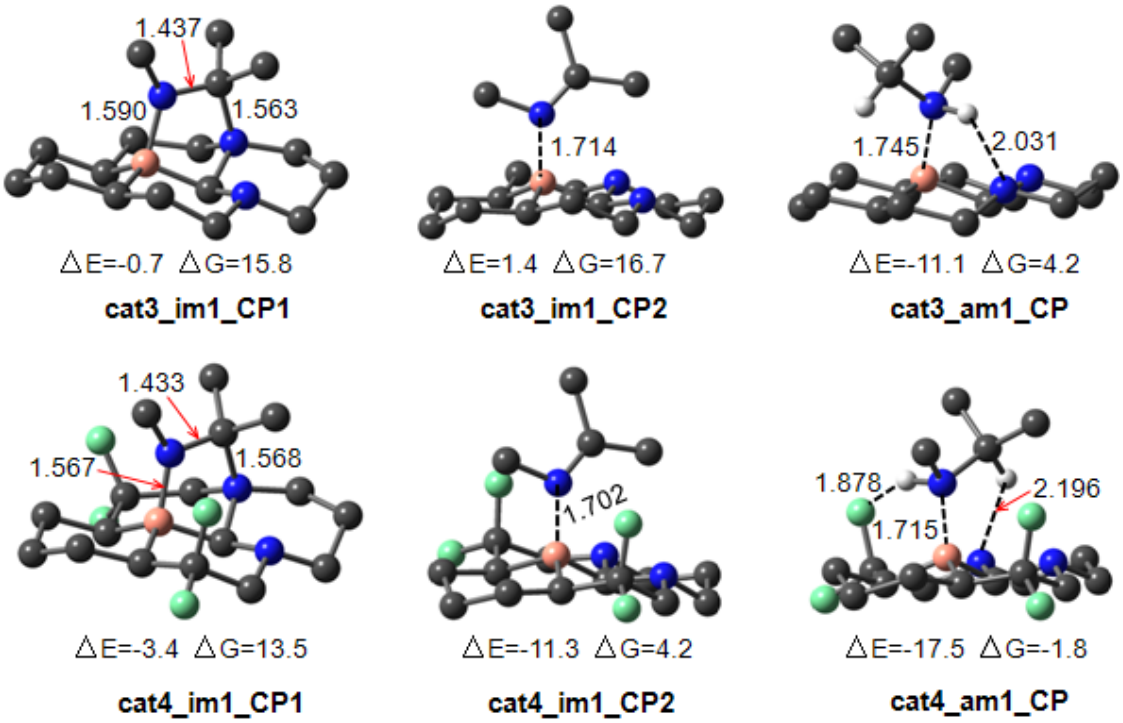

Fig. SI6 M05-2X/6-31G(d,p) optimized structures of various complexes between **cat4**, and **im1** ($MeN=CMe_2$), **am1** ($MeNH\text{-}CHMe_2$).

SI7 The optimized structures for **im1/cat3** hydrogenation

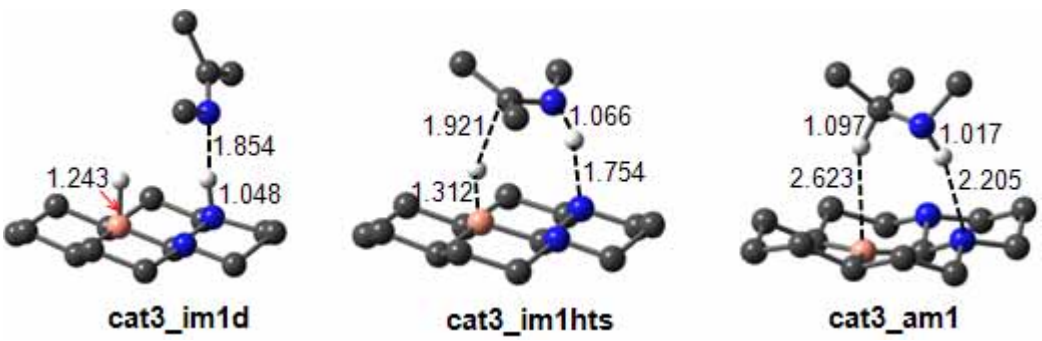

Fig. SI7 Optimized structures of the stationary points along the reaction pathway for **im1/cat3** hydrogenation, along with the key bond distances in Å. Trivial hydrogen atoms are omitted for clarity.

SI8. The optimized geometries at the M05-2X/6-31G(d,p) level and total energies (with ZPE correction) of stationary points in both gas phase and solvent (including the non-electrostatic interactions) at the M05-2X/6-311++G(2d,p) level.

H_2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1.165804	-1.155511	-1.152207	-1.166994

H	0.000000	0.000000	0.370333
H	0.000000	0.000000	-0.370333

im1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-212.600598	-212.474208	-212.466531	-212.504305

N	0.59595700	-0.83754800	-0.00003100
C	-1.78707800	-0.66547000	0.00000400
C	-0.40957800	-0.06090400	0.00000600
C	-0.33519200	1.45133100	0.00000700
H	-2.34660300	-0.33570400	-0.87959500
H	-1.70919500	-1.74995800	-0.00029700
H	0.20507500	1.80975200	-0.87978900
H	-1.32921300	1.89574100	0.00098600
H	-2.34636900	-0.33619200	0.87993700
H	0.20685100	1.80973900	0.87870500
C	1.91796600	-0.22773500	0.00000100
H	2.07935300	0.40028500	-0.88309400
H	2.07978000	0.39886500	0.88403300
H	2.67191600	-1.01302500	-0.00077800

am1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-213.811586	-213.660154	-213.65235	-213.690057

C	0.43933300	-0.01080800	-0.33331600
N	-0.72095200	-0.68638100	0.24292300
H	-0.61330000	-0.71628900	1.25108900
C	-2.00240300	-0.08829500	-0.09698800
H	-2.10913600	-0.08092300	-1.18421200
H	-2.80539200	-0.70504900	0.30855500
H	-2.15023700	0.93978000	0.26101000
H	0.29164200	-0.02015000	-1.41937600
C	1.68236900	-0.83174300	-0.00568500

H	2.56867900	-0.41142600	-0.48342100
H	1.85551600	-0.83577100	1.07489200
H	1.54972100	-1.86190300	-0.33457000
C	0.62054200	1.44234700	0.12002400
H	0.74614400	1.48157200	1.20635600
H	1.50908500	1.88240600	-0.33718500
H	-0.23510200	2.06340800	-0.14780500

***t*BuN=C(H)Ph (*E*-isomer)**

im2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-483.013729	-482.775235	-482.762528	-482.813188

C	-0.23256900	0.53856500	0.00001500
N	-1.11112500	-0.37402000	-0.00000200
C	-2.53939700	-0.04796200	-0.00002200
C	-3.12459900	-0.71219700	1.25112300
H	-2.70880500	-0.25746300	2.15219100
H	-4.21050300	-0.59716100	1.26898600
H	-2.87799600	-1.77429400	1.25605200
C	-3.12459800	-0.71232700	-1.25108700
H	-4.21050200	-0.59731500	-1.26891900
H	-2.70883000	-0.25766400	-2.15220100
H	-2.87797000	-1.77441600	-1.25590900
C	-2.88559800	1.44285800	-0.00006200
H	-2.49725000	1.94627900	0.88830700
H	-2.49722500	1.94629600	-0.88841200
H	-3.97082800	1.55616300	-0.00008800
C	1.21178300	0.22786700	0.00003100
C	1.66586500	-1.09411500	0.00003600
C	2.13568300	1.27279200	0.00001200
C	3.02744500	-1.35995600	0.00001300
H	0.93143400	-1.88889200	0.00007700
C	3.50129900	1.00567500	-0.00002500
H	1.78105400	2.29796200	0.00003800
C	3.94798800	-0.31140200	-0.00003200
H	3.37718700	-2.38489600	0.00002800
H	4.21292500	1.82171100	-0.00003900
H	5.01003800	-0.52315300	-0.00008500
H	-0.47467100	1.60620900	-0.00001800

_t_BuN=C(H)Ph (_Z_-isomer)

	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-482.998328	-482.760001	-482.747221	-482.798365

C	0.37594400	-0.59196900	1.41998400
H	0.21372300	-0.99859100	2.42260600
N	1.58895000	-0.45641900	1.08373400
C	2.06488300	0.04608900	-0.21532900
C	3.44124800	-0.60436800	-0.40090900
H	3.92528700	-0.22718500	-1.30418900
H	4.07100900	-0.38921000	0.46271900
H	3.33751500	-1.68787500	-0.48613400
C	2.24364200	1.56251500	-0.08445200
H	2.83173700	1.79657400	0.80413200
H	2.76307500	1.95143500	-0.96292300
H	1.27553800	2.05946400	-0.00827600
C	1.20015700	-0.28706900	-1.43851600
H	0.94980500	-1.35005900	-1.45291300
H	0.27649100	0.28693200	-1.47423200
H	1.77384900	-0.06188700	-2.34057100
C	-0.89346900	-0.27255800	0.68992500
C	-1.66476300	-1.30149600	0.14684900
C	-1.35693800	1.04190200	0.61521600
C	-2.85929800	-1.01447300	-0.50434700
H	-1.31648900	-2.32506300	0.22130300
C	-2.55630400	1.32759200	-0.03089800
H	-0.77824500	1.83821300	1.06722700
C	-3.30521400	0.30128100	-0.59832500
H	-3.44313800	-1.81726400	-0.93714600
H	-2.90603100	2.35081600	-0.08870800
H	-4.23609600	0.52395400	-1.10422200

am2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-484.224235	-483.961438	-483.94814	-484.001254

C	0.19605900	0.68555500	0.38361000
N	1.08761000	-0.26904900	-0.26090500
C	2.53226000	-0.06983700	-0.06738700
C	3.00375200	1.34869200	-0.41912000
H	2.58292800	2.09069100	0.26219700
H	4.09187900	1.41633400	-0.35262000
H	2.70782100	1.60940300	-1.43896200
C	3.22369100	-1.07670600	-0.98750700
H	4.30692000	-1.03278100	-0.86254400

H	2.87875800	-2.08603100	-0.75883500
H	2.99513200	-0.86129700	-2.03531300
C	2.89519300	-0.39310700	1.38386600
H	2.47529600	0.33559600	2.07948900
H	2.51881400	-1.38275600	1.64630100
H	3.97982700	-0.38001500	1.50895800
C	-1.25121400	0.29754300	0.16949100
C	-1.63764700	-1.04365500	0.18738900
C	-2.22358900	1.27803500	-0.02280600
C	-2.97373000	-1.39315600	0.02363600
H	-0.87489300	-1.80023700	0.31946500
C	-3.56187200	0.93051700	-0.18332700
H	-1.92925700	2.32182500	-0.04937100
C	-3.94048200	-0.40767900	-0.16008200
H	-3.26204700	-2.43736900	0.03838200
H	-4.30546500	1.70365100	-0.33337100
H	-4.98012500	-0.68168300	-0.28959500
H	0.40663400	0.67672600	1.45693200
H	0.88795300	-0.26860200	-1.25588100
H	0.33203500	1.72267500	0.04452900

cat1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-953.446583	-952.938539	-952.921202	-952.979379

C	0.71049400	2.56096300	-0.58938200
C	0.71048300	-2.56095900	-0.58938500
C	2.01446400	-1.27784900	1.24658300
C	2.01446900	1.27784500	1.24658500
C	2.83596500	-0.00000400	1.52384200
C	1.54363300	1.32446500	-0.24450600
C	1.54362800	-1.32446600	-0.24450700
B	0.71346000	0.00000100	-0.24732000
C	2.80016500	-1.25425600	-1.12920100
C	2.80017000	1.25425100	-1.12920000
C	3.63367800	-0.00000400	-0.84182900
C	-0.85612900	0.00000200	0.02831500
C	-2.81923300	1.24214200	-0.69857200
C	-3.29952100	0.00002300	-1.44971200
N	-1.35064000	-1.20486200	-0.68343100
C	-2.81923400	-1.24211700	-0.69860500
C	-3.41114900	1.25155400	0.72038100
C	-1.38403100	-0.00003100	1.49126400
C	-3.41115800	-1.25156700	0.72034400
C	-2.92339900	-0.00002000	1.46426400
N	-1.35064000	1.20488200	-0.68340700
C	-0.75293600	2.43885800	-0.17144800
C	-0.75295000	-2.43884000	-0.17146400

C	4.07594300	-0.00000600	0.62481200
H	1.16271100	-1.33081600	1.93252400
H	1.16271700	1.33081400	1.93252600
H	2.63390900	-2.16341700	1.44092400
H	2.63391800	2.16341000	1.44092600
H	3.14305300	-0.00000500	2.57382300
H	3.40951500	-2.15334000	-0.96245400
H	2.50305100	-1.26324200	-2.18348500
H	3.40952400	2.15333300	-0.96245100
H	2.50305700	1.26324100	-2.18348300
H	4.51591600	-0.00000600	-1.48879900
H	-3.12059600	2.14228400	-1.24185400
H	-4.39125300	0.00002400	-1.51632900
H	-2.87673200	0.00003500	-2.45498900
H	-3.12059700	-2.14224500	-1.24191100
H	-4.50476900	1.25920700	0.66602800
H	-3.10619600	2.15581600	1.25519200
H	-1.02431600	0.87314800	2.03925600
H	-1.02433000	-0.87324600	2.03920800
H	-4.50477800	-1.25920800	0.66598600
H	-3.10621400	-2.15584700	1.25513000
H	-3.30929700	-0.00003500	2.48756800
H	-1.31626000	3.27234500	-0.59959600
H	-0.83576300	2.54210900	0.92008700
H	-1.31627800	-3.27232400	-0.59961400
H	-0.83578900	-2.54208200	0.92007200
H	4.68785400	-0.88354900	0.83385500
H	4.68785800	0.88353400	0.83385600
H	0.73227100	2.68618900	-1.67581000
H	1.14856700	3.46504700	-0.14869800
H	1.14854500	-3.46504400	-0.14869300
H	0.73226700	-2.68618900	-1.67581200

cat1_bts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-954.598704	-954.074507	-954.05735	-954.114831
Imaginary Frequency (one)		ν=1155.7i cm^{-1}		

C	-0.72554200	-2.56269100	-0.53974900
C	-0.72050500	2.53909300	-0.65770200
C	-1.98025000	1.30704200	1.21165100
C	-1.99958300	-1.25459300	1.30823500
C	-2.79688800	0.04404100	1.55870900
C	-1.56089100	-1.33055000	-0.16715600
C	-1.56238000	1.31861200	-0.27907700
B	-0.70906400	-0.01143500	-0.44248200

C	-2.84017900	1.23594600	-1.12792600
C	-2.82881800	-1.28795100	-1.04074800
C	-3.65596600	-0.01992700	-0.78183400
C	0.84518100	0.03512900	0.05370200
C	2.83762200	-1.18985000	-0.75492400
C	3.34227400	0.09960800	-1.40034600
N	1.39235300	1.23779300	-0.60176300
C	2.85374400	1.28825800	-0.56803500
C	3.38955700	-1.29204600	0.67704400
C	1.35183300	-0.05584500	1.50463400
C	3.41214300	1.20247000	0.85980200
C	2.89375600	-0.09166700	1.50032800
N	1.35623800	-1.15027000	-0.72378800
C	0.76943700	-2.42677500	-0.23187100
C	0.72332800	2.46110300	-0.15258500
C	-4.06206300	0.02435800	0.69495200
H	-1.10205100	1.36411700	1.86262400
H	-1.13532800	-1.29036000	1.97877600
H	-2.59093700	2.19526100	1.42833300
H	-2.63341100	-2.11679400	1.56078200
H	-3.07820300	0.08628500	2.61569200
H	-3.45924900	2.13049200	-0.96764600
H	-2.57130000	1.21772000	-2.19081700
H	-3.44722900	-2.17640800	-0.84780000
H	-2.54005400	-1.32143300	-2.09842500
H	-4.55403700	-0.04666900	-1.40696100
H	3.13267200	-2.05810500	-1.34911800
H	4.43466500	0.07769000	-1.44059100
H	2.95052100	0.18780500	-2.41506000
H	3.16654600	2.22063800	-1.04531100
H	4.48300600	-1.28994200	0.63254600
H	3.09011400	-2.23345100	1.14348300
H	0.95400800	-0.92549300	2.02786400
H	1.01103200	0.81599900	2.06621600
H	4.50696000	1.21082900	0.83988000
H	3.08658500	2.06931800	1.44203000
H	3.26069100	-0.17677700	2.52634300
H	1.32021100	-3.23311000	-0.72189300
H	0.93816400	-2.53042400	0.84096400
H	1.28963900	3.30329000	-0.55923200
H	0.74086100	2.57771000	0.94223700
H	-4.66445000	0.91720300	0.89323000
H	-4.67312400	-0.84981100	0.94405700
H	0.42991700	-0.65830000	-1.66217700
H	-0.37263500	-0.15814900	-1.83795100
H	-0.68214200	2.60051200	-1.75036300
H	-1.17704800	3.46870800	-0.29236800
H	-0.83118600	-2.72236200	-1.61844100

H	-1.09288100	-3.47405800	-0.05225900

cat1_c	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-954.636055	-954.104729	-954.087472	-954.145083

C	-0.72962400	-2.54057000	-0.61988300
C	-0.73852700	2.52856800	-0.69653100
C	-1.95580100	1.30468900	1.22810900
C	-1.95350100	-1.27120200	1.27944200
C	-2.74253200	0.02276600	1.58294800
C	-1.56432800	-1.32215500	-0.20730500
C	-1.57906300	1.32262300	-0.26452400
B	-0.73790200	0.00155100	-0.61288600
C	-2.88581400	1.25163800	-1.07195200
C	-2.86777200	-1.28948500	-1.02604600
C	-3.68182100	-0.01884200	-0.72349100
C	0.81408500	0.05622100	-0.04203200
C	2.91659800	-1.21107900	-0.66292200
C	3.43204600	0.07317300	-1.31350400
N	1.41897900	1.22851400	-0.68512400
C	2.87648000	1.28282600	-0.55051500
C	3.35324800	-1.26867800	0.80193800
C	1.26477400	-0.02651000	1.43220300
C	3.35379600	1.23448800	0.90836100
C	2.79975700	-0.04453300	1.54554300
N	1.41690600	-1.17833000	-0.73555300
C	0.75916400	-2.45128100	-0.26576800
C	0.73298200	2.46222400	-0.26418600
C	-4.03866300	0.00423400	0.76609600
H	-1.06880400	1.37423500	1.86475100
H	-1.07666000	-1.32104900	1.93116500
H	-2.58291000	2.17424700	1.47780200
H	-2.58534900	-2.13286800	1.54564100
H	-2.98718400	0.04173100	2.65034600
H	-3.51518400	2.13332700	-0.87493600
H	-2.64878500	1.25247900	-2.14158200
H	-3.48724400	-2.17354900	-0.80827900
H	-2.62318000	-1.31594300	-2.09395900
H	-4.60160200	-0.03886100	-1.31761300
H	3.24582300	-2.09630600	-1.21254000
H	4.52443000	0.06164600	-1.28495500
H	3.11335400	0.12872400	-2.35714900
H	3.22125900	2.19943600	-1.03560200
H	4.44669800	-1.26898300	0.82376600
H	3.02406800	-2.19704000	1.27419400
H	0.84080800	-0.88364700	1.95268400
H	0.87894600	0.85024600	1.95108300

H	4.44806400	1.24901900	0.95076900
H	2.99242600	2.11147000	1.45103800
H	3.09109500	-0.10070500	2.59728500
H	1.31939700	-3.26960400	-0.72408500
H	0.90357000	-2.50841500	0.80854000
H	1.27706600	3.29329800	-0.72196100
H	0.79698500	2.61397800	0.82447300
H	-4.63919400	0.89108100	0.99559400
H	-4.63518900	-0.87726200	1.02627100
H	1.12148200	-1.01849600	-1.70594100
H	-0.53447500	-0.04394700	-1.84224300
H	-0.75588700	2.56811100	-1.79033100
H	-1.15283800	3.47793500	-0.32770300
H	-1.09592900	-3.48126100	-0.18548100
H	-0.80965100	-2.64677100	-1.70775300

cat1_im2d	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1437.65409	-1436.883175	-1436.852179	-1436.94196

C	2.39047400	1.22575900	1.95386700
C	0.83619400	-0.82401000	-2.40985100
C	3.27110700	-1.22195900	-1.64374500
C	4.06987400	-0.19319200	0.57939600
C	4.44698700	-0.58878200	-0.86673900
C	2.89186900	0.79493900	0.57087200
C	2.07626500	-0.25378600	-1.71466200
B	1.64360500	0.16141600	-0.22655100
C	2.55939500	1.02451200	-2.41962200
C	3.33895500	2.03647700	-0.22296400
C	3.73763300	1.66293000	-1.66175700
C	0.83267400	-1.03618400	0.57210000
C	-0.69686400	-1.05023100	2.59203100
C	-1.86225200	-1.30683300	1.63953900
C	-1.36467100	-2.12207800	0.43819500
C	-0.09991300	-2.37142200	3.07579800
C	1.42922700	-2.36130600	1.09382200
C	-0.80771700	-3.46589400	0.93257300
C	0.37814100	-3.18084900	1.86246200
N	0.33607400	-0.28159900	1.81474800
C	1.48000400	0.21386800	2.65990100
C	0.04003300	-1.82760800	-1.56418300
C	4.90268300	0.66900300	-1.61378600
H	2.99046400	-2.16822900	-1.17251800
H	3.83865600	-1.09489900	1.15340300
H	3.62233800	-1.47488900	-2.65611100
H	4.95326200	0.25876100	1.05682600
H	5.27344800	-1.30648800	-0.82917400
H	2.87364600	0.80804900	-3.45245400

H	1.73068700	1.74073200	-2.47463800
H	4.19215800	2.52872000	0.26927400
H	2.51714700	2.76201800	-0.25250600
H	4.05373000	2.56935800	-2.18887300
H	-1.00079500	-0.41497000	3.42785100
H	-2.64073300	-1.85393800	2.17757200
H	-2.28211200	-0.35836600	1.29915500
H	-2.19546600	-2.27426900	-0.25551700
H	-0.88333300	-2.91131100	3.61491700
H	0.71748300	-2.20325700	3.78117400
H	2.30836100	-2.20425400	1.71834400
H	1.77655900	-2.93856900	0.23796800
H	-1.58687400	-4.02669400	1.45940100
H	-0.48181200	-4.07552700	0.08608600
H	0.82275100	-4.11799000	2.20673900
H	1.02777500	0.65628000	3.55075700
H	2.04542400	-0.65920300	2.97119900
H	-0.88520100	-2.08605300	-2.08554000
H	0.61813300	-2.76006600	-1.47934200
H	5.21714900	0.40793000	-2.63007800
H	5.76297000	1.11904000	-1.10584900
C	-2.49399900	1.55193100	-0.76783400
N	-2.70738500	2.12661500	0.34364200
H	0.75726800	1.03691400	-0.29286200
H	-0.11874500	0.53088300	1.38316200
C	-2.00831200	3.36565400	0.70407300
N	-0.35591400	-1.30492700	-0.24627800
C	-0.93462500	3.83815100	-0.27789600
H	-1.36542900	4.08732300	-1.25059400
H	-0.46477400	4.74115600	0.11680100
H	-0.15929000	3.08105000	-0.41692500
C	-1.38402800	3.13779900	2.08487900
H	-1.02635100	4.08147300	2.50155500
H	-2.12366200	2.70590400	2.76106100
H	-0.52734000	2.46402000	2.01219900
C	-3.10643800	4.42991000	0.82653800
H	-3.58408500	4.59031900	-0.14158600
H	-3.86747000	4.10356100	1.53651500
H	-2.67967700	5.37533200	1.16817800
C	-3.28462800	0.37137800	-1.17824200
C	-4.35133900	-0.08613700	-0.39781700
C	-2.97844400	-0.28388700	-2.37088100
C	-5.07904600	-1.19987600	-0.79359000
H	-4.58857500	0.45017600	0.51214400
C	-3.71204900	-1.39748500	-2.77145500
H	-2.15641900	0.07445400	-2.97998000
C	-4.75927000	-1.86041300	-1.98052200
H	-5.90278000	-1.55092200	-0.18428500

H	-3.46529000	-1.90194500	-3.69732700
H	-5.33080300	-2.72673500	-2.29000100
H	-1.73963000	1.88482400	-1.48558900
H	1.82524200	2.15612300	1.82591100
H	3.20497600	1.45117900	2.65659200
H	1.07966600	-1.30656600	-3.36764300
H	0.17236700	0.01958900	-2.63042300

cat1_im2ets	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1437.619623	-1436.849804	-1436.820313	-1436.904549
Imaginary Frequency (one)		ν=1454.2i cm^{-1}		

C	0.34819600	-0.45306200	-2.27435500
C	2.96127300	-0.02358200	2.04251700
C	4.08112900	0.70827600	-0.17227300
C	2.75565700	0.48657300	-2.37084400
C	4.14043000	0.41026600	-1.68760300
C	1.77577200	-0.50215300	-1.71604200
C	3.13750200	-0.27588200	0.54058400
B	1.67323300	-0.22099800	-0.12846900
C	3.68675600	-1.69122500	0.29153300
C	2.37790400	-1.90710800	-1.88731500
C	3.76063100	-2.00398400	-1.21525800
C	0.77432400	1.08462600	0.29293800
C	-1.58909800	1.77036300	0.18304900
C	-1.65140100	1.68029000	1.71342700
C	-0.27365200	2.01991900	2.29832200
C	-1.23004600	3.21154000	-0.20697500
C	1.16577800	2.53601200	-0.11189400
C	0.07034300	3.46990500	1.92212600
C	0.13595800	3.55862400	0.39318000
N	-0.59100500	0.77313200	-0.27572800
C	-0.47641700	0.73257100	-1.75522800
C	2.01088400	1.13302100	2.39846200
C	4.70463400	-1.00042700	-1.88476500
H	3.77014200	1.74420500	-0.01833500
H	2.38501200	1.51293600	-2.32234200
H	5.10209200	0.62866400	0.23433100
H	2.88502400	0.25382900	-3.44031400
H	4.80818000	1.13591000	-2.16489100
H	4.69262400	-1.80771000	0.72614400
H	3.03565400	-2.42308300	0.78547500
H	2.48377000	-2.16356700	-2.95407700
H	1.70473700	-2.65185700	-1.44562000
H	4.15284700	-3.01814800	-1.35188200
H	-2.55675700	1.50337400	-0.25388700

H	-2.39943200	2.38500700	2.08915500
H	-1.94042800	0.67555500	2.02818400
H	-0.30132800	1.90641900	3.38744500
H	-2.00546100	3.88513300	0.17419100
H	-1.21137300	3.32413400	-1.29406100
H	1.29078700	2.65053300	-1.18660400
H	2.13727800	2.77462300	0.31855100
H	-0.69090900	4.14963700	2.32143200
H	1.02895600	3.76186500	2.35853900
H	0.42996700	4.56770000	0.08923800
H	-1.49030700	0.70397500	-2.15788000
H	-0.03295000	1.65341600	-2.14126700
H	1.84524000	1.13219900	3.48167500
H	2.51509900	2.08320200	2.17017600
H	5.70476500	-1.07085700	-1.44268900
H	4.79722800	-1.22425600	-2.95366800
C	-3.07818700	-1.60526400	0.54367300
N	-1.82264200	-1.61984300	0.78720900
H	1.00617100	-1.13985200	0.35985400
H	-1.17992300	-0.83747100	0.32981800
C	-1.22618600	-2.59231600	1.76765300
N	0.68397000	1.04182000	1.76915800
C	-2.29552400	-3.43903900	2.45612400
H	-2.84612200	-4.07722000	1.76062300
H	-1.77416000	-4.09278600	3.15504800
H	-2.99473300	-2.83476000	3.03902700
C	-0.45403500	-1.79696700	2.81730200
H	0.15149500	-2.49154100	3.40246300
H	0.18659100	-1.04526400	2.35393200
H	-1.14991900	-1.29121100	3.49248400
C	-0.31214400	-3.51529900	0.95422400
H	-0.89044700	-4.05835600	0.20283100
H	0.47576600	-2.94194700	0.47077200
H	0.14128600	-4.23857500	1.63413000
C	-3.75451400	-0.84368500	-0.50761400
C	-3.28340900	-0.86559300	-1.82008900
C	-4.95300200	-0.19029600	-0.19625500
C	-3.99387900	-0.20036400	-2.81402600
H	-2.37709200	-1.40794400	-2.05776800
C	-5.63725300	0.49918700	-1.18567100
H	-5.32751200	-0.20374000	0.82068600
C	-5.15713600	0.49175200	-2.49541300
H	-3.63081300	-0.21808200	-3.83339000
H	-6.54812700	1.03046000	-0.94307800
H	-5.70038700	1.01755600	-3.27014300
H	-3.71530900	-2.23689100	1.15213100
H	3.91946100	0.16773300	2.54859400
H	2.55211000	-0.94028600	2.48254100

H	-0.14772500	-1.38529000	-1.96593600
H	0.32279500	-0.42822300	-3.37474300

cat1_im2f	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1437.622017	-1436.852341	-1436.821912	-1436.909216

C	-0.47831100	-0.13199200	-2.41630100
C	-2.76519800	0.49268800	2.06223900
C	-4.05693700	-0.66144600	0.14695400
C	-2.90200700	-0.97572300	-2.13072800
C	-4.22856000	-0.70094500	-1.38776800
C	-1.85481100	0.09554200	-1.78239900
C	-3.04245900	0.42064800	0.55668100
B	-1.63385700	0.16395800	-0.18401900
C	-3.58623400	1.76386200	0.04112800
C	-2.43838900	1.45163100	-2.21475100
C	-3.76531300	1.74215900	-1.48861900
C	-0.73475600	-1.05193200	0.45005100
C	1.59132400	-1.83322900	0.32619800
C	1.77938900	-1.40129200	1.78603200
C	0.44848500	-1.54872200	2.53520800
C	1.17844700	-3.31276000	0.30470700
C	-1.19096400	-2.54105600	0.41603700
C	0.04553000	-3.03215500	2.52389300
C	-0.14382400	-3.46118100	1.06464400
N	0.58027600	-0.93529000	-0.27053900
C	0.35922900	-1.20664600	-1.70749600
C	-1.80395500	-0.58366200	2.59792200
C	-4.77750400	0.65170400	-1.85255100
H	-3.75467700	-1.64850400	0.50320900
H	-2.54894100	-1.97833600	-1.87964800
H	-5.04097700	-0.45680100	0.59881500
H	-3.10626700	-0.98009800	-3.21384300
H	-4.94545300	-1.48914700	-1.64356700
H	-4.55604700	2.00213600	0.50729900
H	-2.89246100	2.56759000	0.31750200
H	-2.61648700	1.47644200	-3.30230300
H	-1.71673900	2.24727200	-1.98998100
H	-4.14630500	2.71554900	-1.81846400
H	2.52870100	-1.70346300	-0.22651400
H	2.54454100	-2.02522700	2.25828600
H	2.10640900	-0.36032500	1.83517000
H	0.56612900	-1.19547800	3.56597700
H	1.96570500	-3.91429400	0.77320300
H	1.07023900	-3.66704200	-0.72404000
H	-1.39378500	-2.88536200	-0.59663100

H	-2.13202000	-2.64918300	0.95349100
H	0.82275600	-3.63262700	3.01029700
H	-0.88068500	-3.18270400	3.08454700
H	-0.48268000	-4.50091100	1.02231200
H	1.34227300	-1.29056500	-2.17754200
H	-0.12323100	-2.17584800	-1.86844800
H	-1.55486100	-0.34612000	3.63880600
H	-2.33847600	-1.54406000	2.62710500
H	-5.73924500	0.85423400	-1.36790500
H	-4.94699800	0.63915000	-2.93538200
C	3.07167700	1.75558700	0.21469800
N	1.81535000	1.87451200	0.43263000
H	-0.90150800	1.14635600	0.03482100
H	1.15913800	1.11459500	0.09411600
C	1.22467500	2.98393100	1.25232300
N	-0.52793300	-0.67782600	1.86971200
C	2.29473900	3.96507000	1.72091300
H	2.81332700	4.44857000	0.88933100
H	1.78265700	4.74308600	2.28680200
H	3.02102600	3.50409700	2.39416500
C	0.53705000	2.33533300	2.45171500
H	-0.08262700	3.08187600	2.95130500
H	-0.07509100	1.49046300	2.12955200
H	1.28541300	1.96858200	3.15952500
C	0.23163700	3.71418900	0.34335500
H	0.74873900	4.15842700	-0.51023700
H	-0.53758900	3.02927700	-0.00933900
H	-0.24034900	4.51224600	0.91856600
C	3.71010800	0.78811700	-0.66692800
C	3.13985500	0.43216800	-1.88990000
C	4.96508400	0.28893000	-0.29539100
C	3.81891600	-0.44321400	-2.72890700
H	2.18500300	0.84851300	-2.18261700
C	5.61829300	-0.61323700	-1.12075800
H	5.40964200	0.59150000	0.64570800
C	5.04490600	-0.97451900	-2.33980700
H	3.38370800	-0.71593100	-3.68149900
H	6.57505000	-1.02323500	-0.82566700
H	5.56300500	-1.66504600	-2.99306800
H	3.72839400	2.45190100	0.72310900
H	0.05900700	0.82583200	-2.35531600
H	-0.54031100	-0.39488100	-3.48363100
H	-3.68875100	0.43639900	2.65821800
H	-2.32359500	1.47444900	2.26749800

cat1_im2gts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1437.614996	-1436.847811	-1436.818489	-1436.901291
Imaginary Frequency (one)		ν= 384.1i cm^{-1}		

C	-1.46935700	0.85494500	2.47845000
C	-0.71192500	-1.65906700	-1.92556000
C	-3.01673500	-1.67332000	-0.80771000
C	-3.37867100	-0.42622900	1.38038000
C	-3.76058500	-1.65584800	0.53952000
C	-1.86189100	-0.38772400	1.67242000
C	-1.48681500	-1.68220500	-0.60326000
B	-1.07495100	-0.40257600	0.27371000
C	-1.15749900	-2.93795600	0.22550000
C	-1.51798500	-1.68723500	2.42189000
C	-1.88973900	-2.92535400	1.58129000
C	-0.98737600	1.01499300	-0.50751000
C	-0.04191000	3.23853100	-0.16969000
C	0.95966900	2.94578700	-1.29208000
C	0.30757700	2.01458900	-2.32052000
C	-1.26301800	3.95016400	-0.77550000
C	-2.26731400	1.68684700	-1.09322000
C	-0.91354100	2.72404300	-2.92724000
C	-1.91033000	3.00856600	-1.79712000
N	-0.37052400	1.95544200	0.47123000
C	-1.23100300	2.13136400	1.65138000
C	-0.55311000	-0.26038800	-2.54595000
C	-3.40026900	-2.91948900	1.32618000
H	-3.33227200	-0.81981900	-1.41151000
H	-3.70425800	0.48262200	0.87032000
H	-3.31225700	-2.57504900	-1.36523000
H	-3.92761100	-0.46249800	2.33369000
H	-4.83951500	-1.63951500	0.35299000
H	-1.43405100	-3.85151500	-0.32230000
H	-0.07802900	-2.98524900	0.39689000
H	-2.04739500	-1.73686300	3.38545000
H	-0.44352500	-1.70601800	2.64875000
H	-1.62097100	-3.82819500	2.14064000
H	0.42479200	3.88524900	0.58178000
H	1.27008200	3.87850600	-1.77164000
H	1.84184800	2.46069500	-0.86804000
H	1.02909600	1.77103700	-3.11030000
H	-0.94211500	4.88090300	-1.25615000
H	-1.97945700	4.22050600	0.00421000
H	-2.99814400	1.89069000	-0.31166000
H	-2.76735600	1.02817900	-1.80171000
H	-0.59934800	3.65679200	-3.40834000
H	-1.37542300	2.10181500	-3.69770000

H	-2.81614900	3.46632900	-2.20565000
H	-0.74219100	2.87346300	2.29386000
H	-2.20801200	2.56263700	1.39642000
H	0.15891900	-0.32822000	-3.37653000
H	-1.51135900	0.03372500	-2.99434000
H	-3.68792100	-3.81164800	0.75948000
H	-3.94472900	-2.93970800	2.27668000
N	-0.03692700	0.76775000	-1.62453000
H	2.88708300	0.86221200	0.16134000
N	2.57494200	0.36710200	0.98262000
C	2.95193300	0.99849100	2.26176000
C	1.97861800	-0.79748600	0.78014000
H	0.27577900	-0.59740000	0.60020000
C	2.52129800	2.46223300	2.20501000
H	1.43598800	2.51486600	2.14274000
H	2.87653000	2.98910200	3.09229000
H	2.94313900	2.95601100	1.32556000
C	4.47593300	0.88709700	2.38960000
H	4.78308000	-0.15979400	2.38657000
H	4.97552500	1.39934500	1.56414000
H	4.80381500	1.34743600	3.32365000
C	2.28460100	0.29206300	3.43314000
H	2.46485300	0.87308300	4.33804000
H	1.21286100	0.22177700	3.27676000
H	2.69426800	-0.70748800	3.59327000
C	2.29179600	-1.54287700	-0.45579000
C	2.42750100	-2.92894700	-0.36795000
C	2.55765800	-0.89764700	-1.66705000
C	2.80501900	-3.66955800	-1.48309000
H	2.22779000	-3.42920600	0.57222000
C	2.93644500	-1.63983900	-2.77654000
H	2.37817100	0.16506300	-1.76098000
C	3.05807100	-3.02589900	-2.68910000
H	2.89819600	-4.74522800	-1.40820000
H	3.11868700	-1.13843900	-3.71874000
H	3.34553900	-3.60035000	-3.56055000
H	1.73797600	-1.37791500	1.65926000
H	0.28123400	-2.06706000	-1.74572000
H	-1.18037700	-2.30852600	-2.67867000
H	-0.56207800	0.62619200	3.03745000
H	-2.23068600	1.09241700	3.23473000

cat1_am2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1437.680728	-1436.908363	-1436.877144	-1436.967201

C	-0.38595700	-1.83515000	2.21902500
C	-0.66391900	-0.16804300	-2.61416000

C	-1.40147200	-2.59272200	-2.05050900
C	-1.26032000	-3.42075900	0.36199500
C	-1.10453900	-3.79439600	-1.12802500
C	-0.27584800	-2.26877400	0.75506900
C	-0.42666100	-1.40785100	-1.74696800
B	-0.80044000	-1.19176100	-0.24642400
C	1.00940200	-1.92645300	-1.93126000
C	1.14988800	-2.75123200	0.43761500
C	1.30205900	-3.13840500	-1.03818300
C	-1.89720000	-0.11660900	0.18840200
C	-2.36419000	1.38009900	2.05331600
C	-2.08143900	2.57325100	1.13984600
C	-2.47936900	2.20323900	-0.28999100
C	-3.86496900	1.05018800	2.02240200
C	-3.40044100	-0.51168000	0.12470900
C	-3.98096000	1.88005500	-0.33854200
C	-4.25523500	0.68313800	0.58383100
N	-1.53971600	0.25928400	1.57782000
C	-1.55529600	-0.88996400	2.48761800
C	-1.80738800	0.71508200	-2.11796800
C	0.33006400	-4.27284100	-1.37651800
H	-2.44770700	-2.28759100	-1.94172800
H	-2.29966200	-3.14602000	0.57030100
H	-1.26598400	-2.89007000	-3.09868500
H	-1.03216500	-4.29393100	0.98711800
H	-1.80675000	-4.59985700	-1.36306100
H	1.16261600	-2.19561100	-2.98589400
H	1.71082900	-1.12164200	-1.69555300
H	1.38548000	-3.61656400	1.07286700
H	1.86939700	-1.96688800	0.68738000
H	2.33066400	-3.46808900	-1.21244800
H	-2.04605200	1.61258000	3.07339600
H	-2.65357200	3.44441900	1.47131100
H	-1.01787700	2.81429100	1.17549400
H	-2.24596700	3.03089000	-0.96749000
H	-4.44119100	1.91593300	2.36467600
H	-4.08865400	0.22232800	2.70116200
H	-3.60218700	-1.37434600	0.76214800
H	-3.68796100	-0.80665800	-0.88579400
H	-4.55529100	2.75243000	-0.01081300
H	-4.29203200	1.65227400	-1.36191000
H	-5.31440000	0.41483200	0.54078700
H	-1.47066000	-0.49527400	3.50352000
H	-2.50061100	-1.45029700	2.45329400
H	-1.79918300	1.65724600	-2.67357800
H	-2.77079700	0.23706400	-2.33857800
H	0.44602400	-4.57239200	-2.42345300
H	0.54272400	-5.14971700	-0.75614000

C	1.72642900	1.59037100	0.83025700
N	1.42237400	1.96269300	-0.54325100
H	0.42716600	1.81951500	-0.69829500
C	1.80915200	3.30494000	-0.99691900
N	-1.65321400	1.05416700	-0.69686000
C	1.45538100	3.37424000	-2.48334600
H	0.38337300	3.20595800	-2.62658500
H	1.70518800	4.35290900	-2.89868900
H	1.99964700	2.60350500	-3.03177400
C	1.05710500	4.42464600	-0.25745700
H	-0.01923200	4.33055300	-0.42392500
H	1.24236900	4.39008600	0.81831000
H	1.37232400	5.40685500	-0.61796500
C	3.31614000	3.50491400	-0.82755500
H	3.61512800	3.43889400	0.22056700
H	3.86840500	2.74854100	-1.38608500
H	3.60287300	4.49144500	-1.19814400
C	2.88307700	0.61530100	0.97371800
C	3.58040900	0.12289600	-0.12640900
C	3.23114900	0.15713800	2.24753200
C	4.59819500	-0.81518700	0.03929400
H	3.29704700	0.47608000	-1.10883000
C	4.24349800	-0.78053500	2.41711300
H	2.69432200	0.53538200	3.11230600
C	4.93079300	-1.27338100	1.30953500
H	5.12778400	-1.19099400	-0.82819000
H	4.49537900	-1.12936500	3.41126800
H	5.71776000	-2.00609200	1.43825300
H	1.93282900	2.46177600	1.46634600
H	0.83522400	1.11391100	1.25535100
H	0.25226200	0.42900300	-2.59101200
H	-0.84679300	-0.44833300	-3.65884800
H	0.53821800	-1.30948900	2.47977200
H	-0.45944800	-2.70678200	2.88116800

cat2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1350.558314	-1350.081523	-1350.061101	-1350.125978

C	-0.56159900	-2.52776700	-0.42001400
C	-0.56166000	2.52775300	-0.41999500
F	-0.62284200	-2.74798800	-1.77104100
F	-1.07568300	-3.66322300	0.16732700
F	-1.07568700	3.66316100	0.16750600
F	-0.62308600	2.74814300	-1.77098600
C	-1.81128200	1.28021900	1.43240200
C	-1.81127000	-1.28030500	1.43237700
C	-2.61814100	-0.00005000	1.73473500
C	-1.40305000	-1.31600300	-0.07917200

C	-1.40307800	1.31595900	-0.07915000
B	-0.56099100	-0.00001500	-0.09853500
C	-2.68788700	1.25636200	-0.92623100
C	-2.68785100	-1.25641400	-0.92625800
C	-3.50287900	-0.00003400	-0.59645500
C	1.01069100	0.00000500	0.16690700
C	2.95672100	-1.24278000	-0.61764800
C	3.41290500	-0.00006100	-1.38269900
N	1.48853300	1.20146000	-0.55661800
C	2.95668800	1.24274100	-0.61780100
C	3.58229800	-1.25216300	0.78595600
C	1.57501800	0.00006900	1.61490400
C	3.58228600	1.25227900	0.78580000
C	3.11380200	0.00009800	1.54201500
N	1.48857400	-1.20149700	-0.55649100
C	0.90253700	-2.42768500	-0.03684400
C	0.90253600	2.42771000	-0.03703100
C	-3.89144200	-0.00001000	0.88454100
H	-0.93445100	1.33382800	2.08486800
H	-0.93445800	-1.33396300	2.08486500
H	-2.41947800	2.16502100	1.64169700
H	-2.41948400	-2.16510500	1.64162400
H	-2.88235400	-0.00006400	2.79563700
H	-3.28397600	2.15585600	-0.73410000
H	-2.42800600	1.26026200	-1.98539900
H	-3.28392000	-2.15593000	-0.73417400
H	-2.42792900	-1.26028400	-1.98541500
H	-4.40754000	-0.00003400	-1.21038100
H	3.23727100	-2.14288900	-1.17053800
H	4.50185600	-0.00005000	-1.48001700
H	2.96190600	-0.00012900	-2.37528300
H	3.23721900	2.14279100	-1.17079200
H	4.67381000	-1.26048600	0.70540300
H	3.29110000	-2.15635100	1.32900600
H	1.23208300	-0.87309100	2.17369400
H	1.23202900	0.87322300	2.17365700
H	4.67379600	1.26057100	0.70521600
H	3.29111500	2.15653200	1.32875400
H	3.52661800	0.00016300	2.55424500
H	1.40435200	-3.27904300	-0.50043100
H	0.97513200	-2.55653100	1.05125200
H	1.40429200	3.27902000	-0.50077000
H	0.97529400	2.55669700	1.05102500
H	-4.49373800	0.88367900	1.11674800
H	-4.49370600	-0.88371100	1.11676900

cat2_bts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1351.713264	-1351.219732	-1351.199499	-1351.263611
Imaginary Frequency (one)		ν= 1149.9i cm^{-1}		

C	-0.58401500	-2.51431100	-0.41643000
C	-0.57898100	2.51422000	-0.43810800
F	-0.69300500	-2.74026200	-1.77104300
F	-1.00970500	-3.67376700	0.18899400
F	-1.11132700	3.68058000	0.07294900
F	-0.57371900	2.67303400	-1.80167400
C	-1.77181500	1.28328900	1.43105800
C	-1.79567000	-1.28432900	1.46820200
C	-2.57324100	0.01196200	1.77809200
C	-1.42515100	-1.31762800	-0.02844300
C	-1.42450500	1.31682400	-0.07792900
B	-0.55955500	-0.00083100	-0.30641800
C	-2.73316200	1.26624700	-0.88381800
C	-2.72611900	-1.26164600	-0.85647400
C	-3.53059200	0.00341900	-0.52155100
C	0.99795800	0.03743700	0.19303600
C	2.96944300	-1.17788300	-0.69178700
C	3.45515700	0.12185500	-1.33195800
N	1.53186700	1.24731100	-0.45624100
C	2.99451800	1.29919500	-0.46774900
C	3.55360200	-1.30392700	0.72460000
C	1.54245900	-0.07527900	1.62778100
C	3.58882100	1.18966600	0.94292100
C	3.08416300	-0.11339800	1.57765500
N	1.48785000	-1.13189200	-0.61861000
C	0.91022500	-2.40310800	-0.13052700
C	0.87385300	2.45643300	0.01731200
C	-3.87470700	0.01540800	0.97042900
H	-0.86658300	1.32294600	2.04380200
H	-0.90509800	-1.33929300	2.10050600
H	-2.36832100	2.16505900	1.68731700
H	-2.41985100	-2.14823500	1.71992500
H	-2.80562000	0.02990000	2.84682700
H	-3.33466900	2.15879900	-0.67420500
H	-2.50673700	1.26791300	-1.95200400
H	-3.33218100	-2.15315900	-0.65432800
H	-2.48557300	-1.26656200	-1.92118800
H	-4.45342400	-0.00742200	-1.10865900
H	3.24175600	-2.03729000	-1.30828900
H	4.54552600	0.09995000	-1.40334200
H	3.03534300	0.22556600	-2.33362100
H	3.29063600	2.23845700	-0.94075100
H	4.64528300	-1.30768700	0.65450400

H	3.26051900	-2.25092200	1.18462400
H	1.15950900	-0.95047100	2.15294100
H	1.22093000	0.78960500	2.21115400
H	4.68231200	1.19544100	0.89409500
H	3.28320300	2.04810300	1.54827400
H	3.47819000	-0.21402600	2.59165500
H	1.39613300	-3.22568600	-0.65645600
H	1.06376100	-2.54121700	0.93917900
H	1.37116700	3.32016900	-0.42753100
H	0.89235700	2.58996400	1.10804200
H	-4.46404000	0.90497400	1.21430300
H	-4.47645200	-0.86276700	1.22566000
H	0.53958100	-0.61117100	-1.52909200
H	-0.25154600	-0.08764400	-1.67819600

cat2_c	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1351.752123	-1351.251356	-1351.231015	-1351.295295

C	-0.57141300	-2.49848100	-0.44818200
C	-0.62263900	2.49723800	-0.47386500
F	-0.60444900	-2.67215900	-1.81594400
F	-0.98937300	-3.69834700	0.08730800
F	-1.10078900	3.67536800	0.07730800
F	-0.69621700	2.67624400	-1.83189100
C	-1.76547100	1.27697300	1.44570000
C	-1.74501100	-1.30296700	1.46474400
C	-2.52672800	-0.01630200	1.80899000
C	-1.42062000	-1.32640100	-0.03928700
C	-1.45293800	1.30544600	-0.06196800
B	-0.59464200	0.00360100	-0.45593900
C	-2.78547700	1.24349600	-0.83145500
C	-2.75027000	-1.30055600	-0.81977500
C	-3.55256400	-0.03733200	-0.45939000
C	0.96618900	0.06266200	0.10306000
C	3.05875900	-1.19301700	-0.58527400
C	3.53695500	0.09494900	-1.25749000
N	1.54258300	1.23832500	-0.55591700
C	3.00449600	1.30379100	-0.47657100
C	3.53863400	-1.24580100	0.86526200
C	1.46579700	-0.01161700	1.56332700
C	3.52953500	1.25943700	0.96524900
C	3.00411400	-0.02183900	1.62292200
N	1.55490200	-1.16770900	-0.60759100
C	0.91867200	-2.42254400	-0.10155400
C	0.86317600	2.45551700	-0.11092200
C	-3.85313100	-0.03479900	1.04191400
H	-0.85436200	1.34440800	2.04627000
H	-0.84110300	-1.35405200	2.07733800

H	-2.38529400	2.13754300	1.72279200
H	-2.35727500	-2.17034700	1.73923900
H	-2.72837300	-0.01205700	2.88469000
H	-3.40547700	2.11859100	-0.59709700
H	-2.58686500	1.25553400	-1.90406100
H	-3.34948500	-2.19064500	-0.58682600
H	-2.54482100	-1.30842800	-1.89132700
H	-4.49343500	-0.05605300	-1.01800700
H	3.37131600	-2.07694800	-1.14553000
H	4.62927600	0.09196000	-1.27059300
H	3.17881900	0.14515000	-2.28822600
H	3.32294300	2.22144900	-0.97624000
H	4.63188800	-1.24365700	0.85472600
H	3.22677800	-2.17468500	1.34897100
H	1.06343200	-0.86379000	2.10878700
H	1.09693300	0.86793900	2.08963900
H	4.62406000	1.27984100	0.97088300
H	3.18334100	2.13526500	1.51985800
H	3.32978000	-0.07318500	2.66435000
H	1.41383600	-3.27051100	-0.57502700
H	1.04742300	-2.48381800	0.97238000
H	1.32413400	3.30829000	-0.61238100
H	0.93682800	2.63026300	0.97116800
H	-4.44955200	0.84483700	1.30474400
H	-4.43242000	-0.92346700	1.31412100
H	1.22664100	-1.03381600	-1.57289700
H	-0.41108400	-0.01498300	-1.67114000

cat2_im2d	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1834.771024	-1834.030329	-1833.996406	-1834.09223

C	-0.18495400	2.19585000	-0.15587800
C	3.04121500	-1.59735700	-0.37024400
F	-0.96510100	1.81207600	-1.23001900
F	-0.45027200	3.53914100	0.02295600
F	4.35300400	-2.04281900	-0.33517100
F	2.46667100	-2.25383800	-1.43367100
C	3.91282100	0.69101800	0.32942500
C	2.25295200	2.66670500	0.44754600
C	3.69531500	2.20827100	0.13495500
C	1.26305900	1.90192800	-0.44692400
C	2.95561500	-0.10500400	-0.57779500
B	1.43256400	0.30388800	-0.25314300
C	3.25173800	0.28421000	-2.03747500
C	1.60676500	2.22061400	-1.91701300
C	3.05296400	1.79858300	-2.23310200
C	0.89039900	-0.29059600	1.19114600
C	-1.40991100	-0.65381600	2.17979900

C	-1.20016100	-2.15466800	1.97317800
C	0.29059600	-2.48252800	2.12468500
C	-0.91833400	-0.23049300	3.56226900
C	1.35433500	0.14509400	2.60008300
C	0.76042300	-2.09387700	3.53407400
C	0.56669000	-0.58198500	3.70244900
N	-0.60530300	0.04142800	1.11020100
C	-0.81424900	1.52224800	1.07068000
C	2.39190000	-2.15033500	0.89800100
C	4.01549000	2.56267200	-1.32038500
H	3.77873800	0.43391900	1.38298100
H	2.04603600	2.51835700	1.50979700
H	4.95449800	0.45266600	0.08382800
H	2.18127800	3.74616700	0.26500400
H	4.37963400	2.74587300	0.79891500
H	4.28158100	0.01550300	-2.30714900
H	2.58209400	-0.26278400	-2.70359000
H	1.49132000	3.29479200	-2.11512300
H	0.92331700	1.68470400	-2.57705700
H	3.26578200	2.04822900	-3.27729200
H	-2.44844200	-0.36826100	2.01922900
H	-1.78649300	-2.69128700	2.72339100
H	-1.55516100	-2.44041300	0.98062600
H	0.44547300	-3.54930900	1.94576200
H	-1.51553100	-0.76925800	4.30326700
H	-1.08683400	0.83575900	3.73334900
H	1.28768000	1.22180200	2.74937000
H	2.41129800	-0.09859200	2.69772600
H	0.18698000	-2.64516400	4.28634200
H	1.81284000	-2.35571700	3.67137700
H	0.92690800	-0.26189100	4.68302200
H	-1.88803600	1.71285500	1.04517800
H	-0.39126900	1.96194100	1.96689900
H	2.42870200	-3.23811400	0.81160900
H	3.03844200	-1.86513200	1.73908800
H	5.05088800	2.29278100	-1.55258900
H	3.90968600	3.64160700	-1.47661400
C	-3.09966000	-0.32181900	-1.73851400
N	-2.55156800	-1.40757600	-1.37642400
H	0.68006400	-0.24888500	-1.04154200
H	-0.90256400	-0.34101600	0.19944300
C	-2.06758000	-2.37488200	-2.37941700
N	0.99645300	-1.74930400	1.06678200
C	-2.81023200	-3.67599800	-2.04985900
H	-3.88806100	-3.54278400	-2.16567400
H	-2.48139800	-4.47477600	-2.71740300
H	-2.60594000	-3.97237500	-1.01973900
C	-0.56448800	-2.57371000	-2.17848900

H	-0.22672400	-3.43064000	-2.76574700
H	-0.00926900	-1.69324800	-2.49849100
H	-0.31414200	-2.74422400	-1.13062000
C	-2.33712800	-1.99109100	-3.83578900
H	-3.40471900	-1.86288900	-4.03201000
H	-1.81098200	-1.07524400	-4.11369500
H	-1.96995200	-2.78965600	-4.48194200
C	-3.75202900	0.57291600	-0.75559300
C	-3.84507500	1.94469300	-1.00053000
C	-4.31576100	0.04250900	0.40765200
C	-4.44802600	2.78293800	-0.06912200
H	-3.40589700	2.35619500	-1.90040600
C	-4.92948100	0.87962200	1.33405400
H	-4.26948800	-1.02925600	0.56050100
C	-4.98790800	2.25234000	1.10078900
H	-4.49564100	3.84827500	-0.25484400
H	-5.37271100	0.46244300	2.23005200
H	-5.46493800	2.90497000	1.82129300
H	-3.15146700	0.00544000	-2.77951100

cat2_im2ets	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1834.747569	-1834.01145	-1833.978475	-1834.069648
Imaginary Frequency (one)		ν= 746.4i cm^{-1}		

C	-0.12306600	-2.09108200	-0.64446200
C	3.11195600	1.46026800	0.68807300
F	-0.74409500	-2.25193500	0.59383300
F	-0.41384500	-3.25954500	-1.32641400
F	4.39682600	1.97681300	0.62225400
F	2.75906700	1.55961900	2.01829700
C	3.84357100	-0.25097600	-1.04843800
C	2.17208400	-2.09562000	-1.73615500
C	3.64996100	-1.71733400	-1.49229600
C	1.35135100	-1.85999200	-0.45432500
C	3.05687200	0.01762100	0.24660300
B	1.49200600	-0.31762300	0.03339400
C	3.59064800	-0.93578500	1.33267200
C	1.94417400	-2.75970500	0.64683500
C	3.42255400	-2.40087400	0.88782500
C	0.67073400	0.77976600	-0.87270600
C	-1.70265700	1.34063400	-1.30486600
C	-1.49257300	2.64138900	-0.51980900
C	-0.04353600	3.11670900	-0.69225300
C	-1.43857700	1.60690300	-2.79060700
C	0.94895800	1.03778000	-2.38229700
C	0.20290700	3.40685200	-2.18042200
C	0.00151600	2.10068600	-2.95759400

N	-0.77200600	0.33025300	-0.72235700
C	-0.89432900	-0.99322400	-1.37314700
C	2.23427200	2.45237900	-0.07763300
C	4.21388700	-2.63340600	-0.40190900
H	3.53711900	0.41945000	-1.85381100
H	1.78487500	-1.52237100	-2.58053600
H	4.91439400	-0.07490000	-0.88851000
H	2.12629900	-3.15209400	-2.02982500
H	4.20444500	-1.87649000	-2.42275500
H	4.65296800	-0.74101700	1.53244100
H	3.04426600	-0.76921100	2.26292400
H	1.87286400	-3.81849200	0.36163900
H	1.38455100	-2.63472500	1.57533900
H	3.81304400	-3.05286600	1.67610300
H	-2.72098100	0.96911300	-1.16785900
H	-2.18009700	3.40215300	-0.89972700
H	-1.70316500	2.48857800	0.53913000
H	0.11933600	4.01737800	-0.09230300
H	-2.15203000	2.36064000	-3.13914100
H	-1.61007300	0.70603900	-3.38561500
H	0.88707500	0.13513300	-2.98637600
H	1.97459100	1.38545700	-2.49442300
H	-0.48944800	4.18059100	-2.52923400
H	1.21690100	3.78476000	-2.33610000
H	0.21901600	2.25781600	-4.01761200
H	-1.94368400	-1.27794300	-1.40460600
H	-0.53551300	-0.97997800	-2.40058600
H	2.29699100	3.39748700	0.46744700
H	2.71379000	2.60797900	-1.05261600
H	5.27444300	-2.41428800	-0.23923600
H	4.13362300	-3.68122100	-0.71141000
C	-3.17976800	0.04090300	1.71001200
N	-1.91303600	0.19443600	1.74217600
H	0.93743200	-0.20870500	1.11069900
H	-1.26461600	0.17430100	0.69909700
C	-1.24305600	0.49553300	3.05727400
N	0.82843000	2.06139100	-0.16206500
C	-2.24061900	0.81205300	4.17358000
H	-2.86282000	-0.04237000	4.44995500
H	-1.65378800	1.08125200	5.05163800
H	-2.87512000	1.66821000	3.93080200
C	-0.31803500	1.69616300	2.87694600
H	0.30652800	1.78951900	3.76683500
H	0.32779200	1.58870700	2.00874400
H	-0.90592100	2.61313300	2.77500200
C	-0.46643000	-0.76929400	3.44030600
H	-1.14736900	-1.61813600	3.53423200
H	0.29033300	-0.99600600	2.69549100

H	0.01889500	-0.59783800	4.40267800
C	-3.99747800	-0.42802500	0.57482000
C	-3.78396400	-1.68936400	0.01752300
C	-5.08455700	0.34992500	0.16224000
C	-4.63408400	-2.14786700	-0.98571300
H	-2.95550400	-2.29402100	0.36215900
C	-5.91140500	-0.10341000	-0.85654700
H	-5.26524500	1.31366000	0.62449400
C	-5.68553800	-1.35370400	-1.43053500
H	-4.46731000	-3.12534000	-1.41969900
H	-6.73667400	0.50970700	-1.19462300
H	-6.33857100	-1.71175500	-2.21612700
H	-3.74359700	0.24428500	2.61493600

cat2_im2f	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1834.755011	-1834.015324	-1833.98176	-1834.074702

C	0.06586000	-0.21269300	2.30525300
C	2.87455000	0.32112500	-1.77248500
F	-0.62419700	1.00093000	2.17253900
F	-0.07942000	-0.53612100	3.64193100
F	4.10701300	0.15734100	-2.38726500
F	2.45803200	1.58134500	-2.16167300
C	3.86737300	-0.89529700	0.22981800
C	2.41762900	-1.16797200	2.34709600
C	3.83642500	-0.96392000	1.77202700
C	1.49738700	-0.02100100	1.89025400
C	2.97502800	0.25665300	-0.26760900
B	1.46368600	0.06047300	0.27008000
C	3.52017000	1.56746100	0.33019400
C	2.09197300	1.29388200	2.42775700
C	3.51269600	1.49988600	1.86916000
C	0.61077100	-1.13202800	-0.47283700
C	-1.75058900	-1.79969000	-0.64138700
C	-1.74172700	-1.31864200	-2.09855500
C	-0.34290700	-1.52365700	-2.69515900
C	-1.41060000	-3.29657000	-0.60960800
C	0.98906900	-2.64225900	-0.42204700
C	-0.01436100	-3.02476600	-2.67485700
C	-0.01696000	-3.49347600	-1.21466600
N	-0.77136700	-0.96889800	0.08805600
C	-0.72901900	-1.25540900	1.52533200
C	1.94227000	-0.68454800	-2.45214300
C	4.40541900	0.34425600	2.32962500
H	3.55523500	-1.85525900	-0.18532400
H	2.03721400	-2.14277200	2.03708100
H	4.90525700	-0.74028000	-0.09023600

H	2.48457500	-1.19129700	3.44259600
H	4.46425400	-1.80029500	2.09600600
H	4.54585500	1.75638500	-0.01532200
H	2.90432500	2.40526200	-0.00310100
H	2.13624600	1.28009700	3.52569200
H	1.46079800	2.13660300	2.13925400
H	3.90819200	2.44236000	2.26242800
H	-2.73612200	-1.63100000	-0.19520200
H	-2.47924300	-1.88346700	-2.67643600
H	-1.99934500	-0.25836900	-2.14571800
H	-0.32044300	-1.14134800	-3.72112200
H	-2.16410700	-3.85192300	-1.17863300
H	-1.43825600	-3.67410900	0.41668700
H	1.04787900	-3.02008300	0.59765000
H	1.98242700	-2.79502600	-0.84262300
H	-0.75747200	-3.57581100	-3.26186200
H	0.96159300	-3.21151500	-3.13092400
H	0.26676800	-4.54861800	-1.16111200
H	-1.74531500	-1.26400700	1.92103100
H	-0.29241100	-2.22808700	1.77186700
H	1.87772600	-0.37741300	-3.49951900
H	2.46097700	-1.65129500	-2.43142300
H	5.42928600	0.49224800	1.97014600
H	4.43818100	0.30509700	3.42401400
C	-3.22167400	1.79493800	-0.45842800
N	-1.94750300	1.91261900	-0.48512900
H	0.81866100	1.05356700	-0.04202000
H	-1.34961600	1.14491300	-0.09052200
C	-1.22732400	3.04763300	-1.14950600
N	0.59110700	-0.72102000	-1.89597700
C	-2.20249800	4.11470600	-1.63557500
H	-2.80020300	4.53416200	-0.82243200
H	-1.60367100	4.92182000	-2.05696300
H	-2.85841100	3.75420900	-2.43119200
C	-0.45260400	2.45895200	-2.32693200
H	0.22375600	3.21850100	-2.72069800
H	0.13333600	1.59133200	-2.02577600
H	-1.14925700	2.16345200	-3.11657400
C	-0.30308600	3.64611200	-0.08629400
H	-0.88374800	4.03276200	0.75390100
H	0.40114500	2.89801400	0.27070400
H	0.25445800	4.46786800	-0.53762900
C	-3.98161700	0.78234000	0.26445100
C	-3.61178700	0.37860400	1.54941000
C	-5.14710400	0.28466500	-0.33169500
C	-4.39832300	-0.55063100	2.22077300
H	-2.72512900	0.79132600	2.01185300
C	-5.90584400	-0.66717600	0.33266400

H	-5.43917000	0.62573200	-1.31816000
C	-5.53091600	-1.08197700	1.61046000
H	-4.12006600	-0.86135200	3.21954700
H	-6.79226500	-1.07551300	-0.13421600
H	-6.13268100	-1.81242100	2.13610400
H	-3.79422500	2.52582300	-1.01759200

cat2_im2g	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1834.738671	-1834.001095	-1833.968231	-1834.058693
Imaginary Frequency (one)		ν= 109.8i cm^{-1}		

C	1.20950400	2.42997400	0.28877500
C	0.76978000	-2.33200600	-1.27054900
F	0.00281000	3.02432500	0.00560600
F	2.09454900	3.49467000	0.38413500
F	1.29569600	-3.38367100	-1.99610000
F	-0.58028800	-2.32729000	-1.59502500
C	2.90470200	-1.08098100	-1.75752900
C	3.12263000	1.33812000	-0.95631000
C	3.48412700	0.31474700	-2.04752500
C	1.58988400	1.48145900	-0.82928700
C	1.36818600	-1.00634400	-1.65335500
B	0.94272600	0.04019200	-0.49947600
C	0.82484800	-0.47669400	-2.99349900
C	1.05196500	1.94128000	-2.19844900
C	1.41534600	0.91579700	-3.28948400
C	1.12766500	-0.47853900	1.03947900
C	0.30141400	0.16151300	3.25180000
C	-0.54552600	-1.11748500	3.28088400
C	0.17063600	-2.21667600	2.48618200
C	1.64721500	-0.13348700	3.93413800
C	2.52034800	-0.76213300	1.67911800
C	1.51933000	-2.51479400	3.15752500
C	2.35993500	-1.23227500	3.13550100
N	0.44601900	0.56705000	1.84389900
C	1.13208200	1.85484300	1.70921400
C	0.86670600	-2.73475200	0.19839800
C	2.93898500	0.80654900	-3.39115200
H	3.34885700	-1.47933900	-0.84304700
H	3.57761900	1.04078100	-0.01001600
H	3.18913800	-1.76247700	-2.56828400
H	3.56015800	2.30726100	-1.22126700
H	4.57446100	0.23572900	-2.10425100
H	1.07925900	-1.15954300	-3.81520400
H	-0.26494700	-0.40874400	-2.94499900
H	1.46977500	2.91964600	-2.47111100
H	-0.03258000	2.05337800	-2.14677700

H	1.01274700	1.26785100	-4.24511300
H	-0.22141800	0.96691000	3.78032400
H	-0.68602100	-1.44254100	4.31546700
H	-1.53215800	-0.92730800	2.85009000
H	-0.45069500	-3.11866800	2.45564800
H	1.47323000	-0.45576300	4.96626700
H	2.26632700	0.76619200	3.97838000
H	3.14579900	0.12910400	1.66362000
H	3.07084400	-1.51724800	1.11852300
H	1.35388900	-2.85168800	4.18638100
H	2.04035000	-3.32121000	2.63393800
H	3.34441400	-1.42710900	3.57039200
H	0.59205500	2.59732100	2.30387300
H	2.16448600	1.83824300	2.07774600
H	0.29260700	-3.65970900	0.30804800
H	1.91612600	-2.98976100	0.38686900
H	3.21678600	0.10880800	-4.18850900
H	3.37056200	1.78261600	-3.63679900
N	0.32039500	-1.72750400	1.10706700
H	-3.53749700	0.02805100	-1.48921600
N	-3.01186300	-0.57449400	-0.86828800
C	-3.57238200	-1.94780500	-0.79357300
C	-2.18306000	0.04256700	-0.06097900
H	-0.35567300	0.15709400	-0.59865800
C	-3.46339600	-2.61263800	-2.16629500
H	-2.42886000	-2.78409600	-2.44344800
H	-3.99198900	-3.56701100	-2.14023400
H	-3.94003100	-1.98914500	-2.92762000
C	-5.05525900	-1.75697900	-0.44344700
H	-5.16329700	-1.23928500	0.51090100
H	-5.57367200	-1.18291500	-1.21603100
H	-5.53745400	-2.73284600	-0.37071700
C	-2.88901100	-2.75164600	0.30347100
H	-3.28087400	-3.76919500	0.27576000
H	-1.81378600	-2.77257700	0.15822700
H	-3.10935400	-2.33129100	1.28791200
C	-2.34239400	1.49980900	0.06941700
C	-2.33602900	2.03866600	1.35563600
C	-2.63581800	2.31175300	-1.02830700
C	-2.64605000	3.38061900	1.54223600
H	-2.08020400	1.40549200	2.19441700
C	-2.92094900	3.65597100	-0.83811400
H	-2.58133500	1.90905100	-2.03459700
C	-2.93515600	4.18954100	0.44880800
H	-2.64819500	3.79733500	2.54140400
H	-3.11947300	4.29091500	-1.69187100
H	-3.15826900	5.23860700	0.59546000
H	-1.66366800	-0.52737400	0.70284300

cat2_am2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1834.796701	-1834.055345	-1834.021111	-1834.116739

C	0.21666800	-0.31235400	2.37973600
C	2.76772700	0.34741000	-1.90484500
F	-0.45704700	0.88412500	2.37129900
F	0.26053900	-0.71015400	3.69741300
F	3.97907500	0.25147800	-2.55216700
F	2.27364700	1.59004700	-2.21611400
C	3.90413400	-0.90885600	0.02451900
C	2.60091600	-1.24400200	2.21032700
C	3.98140700	-0.99209600	1.56483900
C	1.61176200	-0.08728400	1.83689000
C	2.94716400	0.25606800	-0.40481900
B	1.65249000	-0.27555000	0.28759900
C	3.50351400	1.56271100	0.19152200
C	2.22372300	1.23528300	2.33665100
C	3.60949300	1.46546000	1.71928800
C	0.62855200	-1.23661900	-0.47024000
C	-1.77149800	-1.69429200	-0.50548100
C	-1.84064400	-1.10888300	-1.91640300
C	-0.50947700	-1.36148400	-2.62526900
C	-1.53263000	-3.20894800	-0.59056300
C	0.92473500	-2.76367600	-0.53058500
C	-0.26222100	-2.87439100	-2.73046700
C	-0.20203000	-3.46090800	-1.31239100
N	-0.67301000	-1.00346100	0.19859500
C	-0.62426800	-1.32188800	1.62034600
C	1.83424400	-0.68094400	-2.51784600
C	4.55074300	0.32233400	2.10560400
H	3.58250800	-1.86878200	-0.38710300
H	2.21447100	-2.21959700	1.90361000
H	4.89562400	-0.70042000	-0.38839100
H	2.69734300	-1.26735600	3.29978500
H	4.64360300	-1.81985700	1.83244800
H	4.49114500	1.75685700	-0.24241900
H	2.86026100	2.39851600	-0.08143700
H	2.30109600	1.20007900	3.42943000
H	1.56513300	2.06567100	2.08485900
H	4.00707400	2.40971100	2.10068200
H	-2.69557900	-1.47788100	0.03336700
H	-2.65549000	-1.58112000	-2.47188100
H	-2.02856900	-0.03679500	-1.86235300
H	-0.52234000	-0.90027400	-3.61661700
H	-2.35871800	-3.67738300	-1.13409100
H	-1.51261200	-3.65214300	0.40960000

H	0.99374000	-3.19285800	0.47070100
H	1.88363700	-2.96129100	-1.01376900
H	-1.07081200	-3.34072400	-3.30159200
H	0.67033400	-3.07678300	-3.26571200
H	0.00098000	-4.53398500	-1.36223600
H	-1.63717600	-1.25971200	2.02124800
H	-0.23417500	-2.32135300	1.85236500
H	1.68140500	-0.37999000	-3.55611400
H	2.35714300	-1.64609600	-2.52845600
H	5.54756600	0.49620600	1.68878400
H	4.65022400	0.26563400	3.19400100
C	-3.43622600	1.95730400	-0.58957700
N	-2.06671600	2.14215200	-0.14554800
H	-1.59147600	1.24263400	-0.09957900
C	-1.24014400	3.10060400	-0.88785700
N	0.54378200	-0.68974000	-1.84360600
C	-0.98816100	2.69331400	-2.34845700
H	-1.92320800	2.60746000	-2.90769300
H	-0.37031400	3.44322800	-2.84905000
H	-0.45474200	1.74031000	-2.38154000
C	0.09885600	3.13775700	-0.15346600
H	0.80838200	3.79081700	-0.66604500
H	-0.04683000	3.47845900	0.87277400
H	0.52290100	2.12924000	-0.13180000
C	-1.89196300	4.48335000	-0.83296200
H	-2.78182200	4.53524200	-1.46424300
H	-2.17574500	4.71977500	0.19446900
H	-1.18978700	5.23982100	-1.18902700
C	-4.09408100	0.84501400	0.19781300
C	-3.75586700	0.62279500	1.53494900
C	-5.04007600	0.01566800	-0.40587400
C	-4.35677500	-0.41084100	2.24918700
H	-2.99693600	1.24527900	1.99081200
C	-5.64016200	-1.01898900	0.30686900
H	-5.29746600	0.17505700	-1.44764100
C	-5.29776900	-1.23679100	1.63845200
H	-4.08549300	-0.57317000	3.28590700
H	-6.36859900	-1.65715000	-0.17847800
H	-5.75970300	-2.04301100	2.19492900
H	-3.98894900	2.88673600	-0.41806800
H	-3.54266800	1.72568600	-1.66171600

cat3	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-643.689655	-643.33005	-643.31591	-643.368604

C	-0.67076500	-2.52015300	-0.22772600
C	-0.67072700	2.52017600	-0.22771300
C	-1.52619000	-1.36142400	0.29264100

C	-1.52617000	1.36147000	0.29264700
B	-0.74800400	0.00001300	0.26162800
C	-2.91819500	1.26770200	-0.34612200
C	-2.91826300	-1.26772500	-0.34598500
C	-3.66340500	0.00003500	0.08302200
C	0.82924700	-0.00000900	0.37688200
C	2.84723400	-1.24490500	0.04325000
C	3.50629200	-0.00001900	-0.53389600
N	1.41478000	1.20413500	-0.21335600
C	2.84725200	1.24487100	0.04326300
N	1.41476400	-1.20414500	-0.21338000
C	0.76274700	-2.41133700	0.28052500
C	0.76278000	2.41133000	0.28055900
H	-3.50836700	2.15729900	-0.10475500
H	-2.80576200	1.25666900	-1.43678900
H	-3.50844600	-2.15726100	-0.10442300
H	-2.80594500	-1.25686300	-1.43666500
H	-3.78259300	0.00009800	1.17316500
H	-4.66937900	0.00003700	-0.34372700
H	3.26193300	-2.14556100	-0.41588400
H	4.57514800	-0.00002600	-0.30948400
H	3.37266600	-0.00001400	-1.61702700
H	3.26196200	2.14552400	-0.41586800
H	1.34484400	-3.26615700	-0.07140900
H	0.77272700	-2.44901200	1.38736400
H	1.34490200	3.26614400	-0.07134500
H	0.77273300	2.44898500	1.38739900
H	-1.09712400	3.48546300	0.06287200
H	-0.64209700	2.49075000	-1.32088800
H	-0.64215900	-2.49073800	-1.32090100
H	-1.09718600	-3.48542300	0.06288100
H	3.04978900	-1.29814700	1.13067800
H	3.04981900	1.29810000	1.13068900
H	-1.66767300	-1.51632900	1.37930300
H	-1.66780700	1.51641500	1.37927200
H	1.05018700	-0.00002100	1.48645900

cat3_bts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-644.834319	-644.457906	-644.443996	-644.495765
Imaginary Frequency (one)		ν= 1240.1i cm^{-1}		

C	0.77052300	2.54919900	-0.00495100
C	0.57773000	-2.54179000	-0.23219600
C	1.56476100	1.31168300	0.42744600
C	1.48631500	-1.39888000	0.21885000
B	0.72304900	-0.00938200	0.10909900
C	2.84360500	-1.31964400	-0.48176900

C	2.93114700	1.22358600	-0.26537300
C	3.64409400	-0.10660300	0.01282400
C	-0.82775200	-0.00357200	0.55117900
C	-2.78678400	1.29754800	-0.24524900
C	-3.45240400	-0.01195200	-0.64403500
N	-1.47128600	-1.18434100	0.01213800
C	-2.90776500	-1.15852800	0.20171000
N	-1.31962200	1.18076500	-0.20767500
C	-0.71651500	2.42669400	0.32997700
C	-0.80308900	-2.41863700	0.41729500
H	3.42372500	-2.23720600	-0.33025100
H	2.68310200	-1.22220700	-1.56323200
H	3.57632100	2.06163500	0.02229600
H	2.77305800	1.30795400	-1.34900300
H	3.81031500	-0.20656700	1.09216200
H	4.63134400	-0.09608200	-0.45716300
H	-3.04798400	2.09914900	-0.93907400
H	-4.53338500	0.08968300	-0.52560000
H	-3.23483300	-0.22932200	-1.69129500
H	-3.33305200	-2.10612900	-0.13505800
H	-1.27002200	3.26504600	-0.09770600
H	-0.87341100	2.44394200	1.41608100
H	-1.43782600	-3.25004800	0.10188900
H	-0.70336600	-2.48537400	1.51522300
H	1.00484200	-3.52179900	0.00971400
H	0.44271500	-2.49804000	-1.31795600
H	0.86583600	2.66681700	-1.09025800
H	1.15177800	3.47217400	0.44386300
H	-3.12949900	1.59390700	0.75687800
H	-3.19015800	-1.01965000	1.26182900
H	1.72752200	1.35309900	1.51455600
H	1.68025000	-1.53631100	1.29647400
H	-1.04281000	0.14301300	1.62757900
H	0.41258300	0.18952100	-1.30689800
H	-0.40913400	0.70010700	-1.14603100

cat3_c	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-644.877154	-644.493649	-644.479545	-644.531744

C	-0.72854700	-2.53369100	-0.17931300
C	-0.68172200	2.52320500	-0.30018400
C	-1.52529800	-1.33513700	0.33393200
C	-1.52009100	1.36762300	0.24333200
B	-0.76928000	0.00508800	-0.15577300
C	-2.95176500	1.29294300	-0.28753900
C	-2.95927100	-1.27905200	-0.19705900
C	-3.65985400	0.02513100	0.22033200
C	0.76763000	0.04736300	0.35519700

C	2.88912800	-1.25385300	0.01738800
C	3.56927300	0.04822000	-0.37808100
N	1.46194700	1.20918100	-0.15621000
C	2.85435400	1.23862800	0.25470600
N	1.42427900	-1.18827400	-0.24396200
C	0.73903400	-2.44023500	0.23493400
C	0.75533600	2.44364500	0.22264900
H	-3.54218100	2.17580100	-0.01033100
H	-2.91931300	1.26275800	-1.38406700
H	-3.55686500	-2.13840700	0.13441300
H	-2.92436300	-1.31944300	-1.29348700
H	-3.70477600	0.06394400	1.31579800
H	-4.69476900	0.01156200	-0.13446800
H	3.29683800	-2.11331100	-0.51752500
H	4.61401600	0.00187300	-0.06490200
H	3.54464100	0.16361400	-1.46413600
H	3.31232000	2.16710700	-0.09214300
H	1.32751600	-3.27831000	-0.14397200
H	0.82855700	-2.41691600	1.32340800
H	1.34576800	3.27630700	-0.16914100
H	0.74118700	2.54634200	1.32289600
H	-1.08250900	3.50799700	-0.02686700
H	-0.65611700	2.46888100	-1.39323500
H	-0.78776100	-2.56491500	-1.27339300
H	-1.09496600	-3.50149200	0.18618300
H	2.98872900	-1.43010800	1.09097200
H	2.96129700	1.20245100	1.35504500
H	-1.56373900	-1.39105900	1.43412900
H	-1.57114100	1.47062800	1.34058500
H	0.92140800	-0.07760700	1.44622200
H	-0.66812900	-0.05673100	-1.39884800
H	1.23792900	-1.07149300	-1.24482500

cat3_im2d	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1127.897647	-1127.274435	-1127.24682	-1127.330309

C	-0.91038500	-1.92172400	-1.71816000
C	-3.60978000	0.91046500	1.48577200
C	-2.35328800	-1.70263500	-1.26633800
C	-3.79833300	-0.18232200	0.43543300
B	-2.34094600	-0.55853500	-0.12782000
C	-4.67366800	0.20998500	-0.75511100
C	-3.29476200	-1.23893000	-2.37902000
C	-4.68831700	-0.89936800	-1.82177200
C	-1.34943900	-0.93198100	1.09437200
C	1.05362700	-1.43271200	1.54076000
C	1.03749400	-0.34141100	2.59911900
C	-0.37065900	-0.16483500	3.16000100

N	0.03252400	-1.13918700	0.49707000
C	-0.01625300	-2.24363500	-0.52198100
C	-2.62655300	0.46052800	2.57076500
H	-5.70472200	0.43898400	-0.45495200
H	-4.26211000	1.12324900	-1.20374100
H	-3.39304600	-1.98578000	-3.17816400
H	-2.87132200	-0.33568600	-2.83764500
H	-5.35087200	-0.61285400	-2.64422100
H	2.02645500	-1.52782400	1.05850200
H	1.74235300	-0.60722700	3.38929800
H	1.36328800	0.60036200	2.15041400
H	-0.38401700	0.66110300	3.87497400
H	1.01601300	-2.43832900	-0.81202900
H	-0.39729900	-3.11747200	0.01259200
H	-2.50387400	1.24863300	3.31890400
H	-3.05099300	-0.41720900	3.09227600
C	2.74802300	1.50577100	-0.50375100
N	1.49543700	1.54468600	-0.69848200
H	-1.84124100	0.46013500	-0.63537300
H	0.28158600	-0.25735900	0.01731900
C	0.79911200	2.84205000	-0.79847100
N	-1.28124900	0.13872100	2.06950800
C	1.71749700	4.05643900	-0.95509500
H	2.37762900	3.95247600	-1.81996400
H	1.09757900	4.94075200	-1.10887000
H	2.32355200	4.23682600	-0.06415200
C	-0.04865500	2.99358200	0.46773400
H	-0.68076300	3.88023000	0.38063300
H	-0.67960100	2.11840100	0.62583400
H	0.59882600	3.11673900	1.34103400
C	-0.10831500	2.72657700	-2.02737200
H	0.49128200	2.59279300	-2.93084900
H	-0.78193200	1.87692300	-1.91438100
H	-0.70285100	3.63589100	-2.13636700
C	3.47554100	0.21775100	-0.46984800
C	3.10475200	-0.82046500	-1.32796100
C	4.54181900	0.03622900	0.41302000
C	3.77878400	-2.03632200	-1.28357900
H	2.29419400	-0.65277100	-2.02731100
C	5.20148500	-1.18722500	0.47099500
H	4.84172900	0.84944800	1.06451600
C	4.82003000	-2.22460000	-0.37639800
H	3.49727500	-2.83474100	-1.95932600
H	6.01598300	-1.32933700	1.16990100
H	5.34174800	-3.17252100	-0.33965300
H	3.35760800	2.40086800	-0.35572400
H	-0.53765000	-1.01123900	-2.20404800
H	-0.79052700	-2.74264800	-2.43728300

H	-4.54714800	1.19411300	1.98236900
H	-3.21068900	1.80967700	1.00406800
H	-5.11616900	-1.80626700	-1.37685200
H	-4.26162400	-1.05396100	0.92774900
H	-2.73375400	-2.65719900	-0.86677500
H	-1.56294600	-1.90398800	1.58628700
H	-0.67432100	-1.08135100	3.70088300
H	0.77158400	-2.39596100	1.97387500

cat3_im2ets	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM	-1127.864561	-1127.244912	-1127.218473	-1127.298134
Imaginary Frequency (one)		ν= 396.7i cm^{-1}		

C	0.03377900	-2.28897700	-1.59993200
C	-3.30693400	0.62482500	0.82628200
C	-1.45097000	-1.95339300	-1.56872400
C	-3.20389000	-0.40800700	-0.28970200
B	-1.64829800	-0.79555400	-0.45941200
C	-3.73249100	0.04392200	-1.65066500
C	-2.03225200	-1.44932800	-2.88887000
C	-3.50663300	-1.04238600	-2.71761500
C	-1.03337400	-1.26008900	0.96169800
C	0.91039000	-2.11820700	2.11026500
C	0.72125400	-1.06935900	3.19574300
C	-0.75317200	-0.70287800	3.29929500
N	0.42713800	-1.59894200	0.81563300
C	0.51390600	-2.68559500	-0.19897700
C	-2.66637800	0.08824200	2.11028500
H	-4.80039200	0.30169400	-1.62004800
H	-3.19371200	0.95185300	-1.95084400
H	-1.95256700	-2.19300800	-3.69436200
H	-1.45957300	-0.56907800	-3.20896600
H	-3.91059800	-0.70808200	-3.67871200
H	1.95539000	-2.41686900	2.03525300
H	1.08436300	-1.45769300	4.14981400
H	1.30525800	-0.17623500	2.95027100
H	-0.90092100	0.09193300	4.03614300
H	1.54867600	-3.03947100	-0.21805700
H	-0.09662800	-3.52931100	0.15273100
H	-2.75881600	0.82038600	2.92010300
H	-3.23130000	-0.80830200	2.42718400
N	-1.23773800	-0.25176400	2.00437100
N	2.21788000	0.16568500	-0.25101400
C	3.52919800	-0.48673400	-0.60664900
C	2.03878400	1.37637800	-0.65557300
H	-1.01031100	0.20401400	-0.83481700
C	3.39947800	-1.23007800	-1.93725400

H	3.09911100	-0.54170200	-2.73014400
H	4.36763100	-1.66049300	-2.20092000
H	2.66511600	-2.03061600	-1.88269300
C	3.89394400	-1.45221700	0.51996500
H	3.88084500	-0.94520300	1.48698900
H	3.21502400	-2.29832900	0.55141800
H	4.89778800	-1.84077800	0.34580300
C	4.66674100	0.54087000	-0.71247000
H	5.60921300	-0.00512100	-0.75021200
H	4.62097600	1.14370700	-1.62012000
H	4.68832900	1.19973100	0.15791400
H	-4.07947900	-1.93295900	-2.43086500
H	-2.00017200	-2.86405900	-1.27562700
H	-3.77937800	-1.29769500	0.01972900
H	-1.50788900	-2.21151500	1.30497000
H	0.32947400	-3.01605800	2.36586000
H	-1.31978400	-1.58780200	3.64636800
H	1.37842900	-0.50169400	0.27209100
H	2.81401900	1.77915400	-1.29967700
C	1.01892100	2.35759600	-0.34747300
C	1.11466400	3.56878600	-1.05317500
C	0.05877700	2.20496600	0.65667700
C	0.25254700	4.61499700	-0.77095600
H	1.86745400	3.68287600	-1.82560200
C	-0.78168300	3.27016100	0.95274300
H	-0.06877000	1.26980400	1.19428900
C	-0.69203400	4.46502700	0.24372700
H	0.32031800	5.54213000	-1.32448500
H	-1.52100200	3.15409500	1.73458200
H	-1.35966700	5.28417700	0.48087400
H	-2.79048900	1.53731200	0.51398200
H	-4.34296200	0.90320200	1.06558200
H	0.57911600	-1.40141400	-1.93943000
H	0.29298200	-3.11078900	-2.28410100

cat3_im2hts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM	-1127.855072	-1127.236975	-1127.210677	-1127.288649
Imaginary Frequency (one)		ν= 838.6i cm^{-1}		

C	1.42391200	-2.50868200	-1.05697400
C	-2.71131300	-0.48284300	1.12262100
C	-0.06873400	-2.75366600	-0.87795300
C	-2.24264600	-1.63184900	0.23159000
B	-0.66701400	-1.58204100	0.02422400
C	-2.94766100	-1.77075800	-1.11880700
C	-0.85764900	-2.82496800	-2.18795300
C	-2.36852200	-2.94364600	-1.92763800

C	0.12833400	-1.33222000	1.39426900
C	2.37435900	-0.84236100	2.26639900
C	1.78372500	0.33261100	3.03024400
C	0.31471800	0.06781400	3.34039800
N	1.57020600	-1.08775700	1.04758700
C	2.12722700	-2.23621900	0.27426600
C	-1.83982700	-0.37291000	2.37597800
H	-4.02839000	-1.91056100	-0.99626000
H	-2.81443600	-0.84267600	-1.68627900
H	-0.52518600	-3.65805500	-2.81884000
H	-0.66876100	-1.90389400	-2.75687500
H	-2.89761300	-3.03245200	-2.88062100
H	3.40693800	-0.65301600	1.97001300
H	2.34964000	0.48582700	3.95094400
H	1.86661400	1.22992500	2.41293800
H	-0.12601600	0.93759200	3.83310400
H	3.18655000	-2.01858800	0.11769800
H	2.05546800	-3.11512800	0.92491200
H	-2.16262300	0.48570500	2.97046500
H	-1.98498700	-1.27488200	3.00102700
N	-0.40757900	-0.18618300	2.10458100
N	1.48093600	1.05885500	-0.47868500
C	2.65991600	1.34149500	-1.32127500
C	0.30212500	0.90591500	-1.08875300
H	-0.32295300	-0.42768600	-0.71443000
C	2.96773800	0.34828700	-2.45250300
H	2.10499900	0.17323300	-3.09908000
H	3.76686600	0.74966600	-3.07997500
H	3.30793200	-0.61025100	-2.05814100
C	3.86441700	1.38844900	-0.37980000
H	3.66532800	2.08083000	0.44010800
H	4.06268600	0.39810800	0.03979600
H	4.76228200	1.71304500	-0.91021500
C	2.46348200	2.73789100	-1.93375400
H	3.36290400	3.06867500	-2.45968700
H	1.63287600	2.72999400	-2.64435700
H	2.22444200	3.45202100	-1.14423400
H	-3.74978600	-0.61947900	1.44773900
H	-2.66722100	0.46129300	0.58025500
H	1.55330800	-1.64678600	-1.71152900
H	1.94621400	-3.34878400	-1.53046900
H	-2.55523900	-3.87402300	-1.37792400
H	-0.21262000	-3.70194800	-0.33297800
H	-2.41763200	-2.57084500	0.78887700
H	0.13466000	-2.23278500	2.05253500
H	2.34192000	-1.75710000	2.86888400
H	0.23085600	-0.78964400	4.03611500
H	1.58806900	-0.12848900	0.42533100

H	0.28834200	0.70114000	-2.16823600
C	-0.87056800	1.74327500	-0.68990600
C	-1.96473400	1.83415000	-1.54998700
C	-0.85243900	2.49725100	0.48253800
C	-3.05508800	2.63315700	-1.22274700
H	-1.96247000	1.26672700	-2.47491500
C	-1.94559000	3.28806600	0.81544900
H	0.02374000	2.44076600	1.11232300
C	-3.05174100	3.35276300	-0.03107900
H	-3.90249900	2.69441200	-1.89408100
H	-1.93451900	3.86481600	1.73249900
H	-3.90019500	3.97308100	0.23032700

cat3_im2f	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1127.869768	-1127.247914	-1127.220907	-1127.30261

C	-0.21726400	-2.63645900	-1.03930000
C	-3.44143700	1.07632500	0.28690000
C	-1.61241300	-2.08990500	-1.32648300
C	-3.29117900	-0.13543300	-0.63007300
B	-1.81380800	-0.75366000	-0.45016800
C	-3.55065000	0.11739900	-2.11602700
C	-1.90601000	-1.75764700	-2.78876300
C	-3.31668700	-1.16043500	-2.94248700
C	-1.47735400	-1.00322000	1.10412400
C	0.25894700	-1.74918100	2.61596000
C	0.11828900	-0.44416600	3.38935400
C	-1.30430900	0.08425900	3.25468100
N	-0.10577600	-1.52804800	1.22251500
C	-0.01126300	-2.79055100	0.47251600
C	-3.01781800	0.73218700	1.71992800
H	-4.56730800	0.48868000	-2.30551300
H	-2.86381300	0.89585800	-2.47653700
H	-1.81203500	-2.63321500	-3.44603400
H	-1.16989000	-1.02018600	-3.13693000
H	-3.52049500	-0.95844200	-3.99907700
H	1.29071000	-2.11702900	2.66457200
H	0.36882300	-0.59745600	4.44159100
H	0.81229000	0.29304000	2.97275600
H	-1.40621100	1.04673600	3.76693600
H	0.97359600	-3.22335900	0.68394700
H	-0.75545000	-3.50880000	0.85985400
H	-3.11578600	1.61568800	2.36119300
H	-3.71226700	-0.03027800	2.11865000
C	2.40876500	1.59096500	-0.49192100
N	1.14683600	1.72377100	-0.29453400
H	-0.94679900	0.08197000	-0.85385400

C	0.41826100	3.03041700	-0.34190300
N	-1.63388300	0.25484200	1.84718300
C	1.37371600	4.20394400	-0.52265300
H	1.88777400	4.18314200	-1.48638000
H	0.77111100	5.11176100	-0.49578300
H	2.10427900	4.27073000	0.28683200
C	-0.32122200	3.15164600	0.99121100
H	-1.01208200	3.99466200	0.93827800
H	-0.87211800	2.23264600	1.21060400
H	0.39114400	3.33239400	1.80017900
C	-0.54559700	2.95351600	-1.52874800
H	0.01145800	2.90306200	-2.46677000
H	-1.18098200	2.07321000	-1.45286400
H	-1.16776000	3.84978100	-1.53681200
C	3.20879600	0.38444100	-0.46302200
C	4.53060600	0.51183100	-0.91754200
C	2.72824100	-0.84715600	0.00056400
C	5.36842800	-0.59112700	-0.93387500
H	4.89179500	1.47375900	-1.26358900
C	3.58208600	-1.94261700	-0.01333100
H	1.70848200	-0.93990700	0.38081900
C	4.88916100	-1.81910400	-0.48095800
H	6.38500400	-0.49800700	-1.29177800
H	3.22564200	-2.90004000	0.34213700
H	5.54017000	-2.68441500	-0.48774600
H	2.94902200	2.50353100	-0.71424900
H	-4.47064900	1.45896600	0.32329500
H	-2.81822500	1.90123600	-0.07592900
H	0.53170000	-1.93833700	-1.43404400
H	-0.02657900	-3.61007200	-1.51155100
H	-4.04578100	-1.91503000	-2.62266600
H	-4.01947000	-0.89184800	-0.29143000
H	-2.34252200	-2.84912500	-0.99886000
H	-2.00114700	-0.62541800	3.73951000
H	-2.16408900	-1.75987000	1.56534200
H	-0.39010800	-2.51772200	3.07433300
H	0.52480500	0.90247700	-0.14663900

cat3_im2gts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1127.865387	-1127.243945	-1127.21755	-1127.296217
Imaginary Frequency (one)		ν= 32.9i cm^{-1}		

C	1.34291100	-2.37871900	-0.69343000
C	-3.26255900	-0.18798900	-0.46792000
C	-0.01237900	-2.32302900	-1.39067000
C	-2.41068900	-1.16568900	-1.27359000
B	-0.92712900	-1.22516900	-0.65334000

C	-2.31852900	-0.90234900	-2.77728000
C	0.01820100	-2.00583900	-2.88548000
C	-1.40788900	-1.93844900	-3.46224000
C	-0.97675900	-1.47498900	0.93646000
C	0.37452100	-1.72674900	2.91627000
C	-0.45604900	-0.65542900	3.61130000
C	-1.85992900	-0.63054900	3.02261000
N	0.39015100	-1.48407900	1.48019000
C	1.17225100	-2.54212900	0.82126000
C	-3.16227900	-0.47876900	1.03300000
H	-3.30335900	-0.91039900	-3.26412000
H	-1.89560900	0.09745100	-2.94680000
H	0.60302100	-2.73837900	-3.45852000
H	0.50657100	-1.03131900	-3.02844000
H	-1.36391900	-1.73593900	-4.53735000
H	1.40294100	-1.72604900	3.29572000
H	-0.50307900	-0.85000900	4.68534000
H	0.01468100	0.32286100	3.46600000
H	-2.45268900	0.17410100	3.46981000
H	2.15585100	-2.56591900	1.30425000
H	0.69684100	-3.52119900	1.01742000
H	-3.75956900	0.24865100	1.59417000
H	-3.60150900	-1.47369900	1.23001000
N	-1.79720900	-0.43273900	1.57912000
H	-0.35728900	-0.06897900	-0.82820000
H	-4.32463900	-0.22110000	-0.74605000
H	-2.92843000	0.83748100	-0.64479000
H	1.89285100	-1.45615900	-0.89277000
H	1.97184100	-3.20664900	-1.04829000
H	-1.86945900	-2.92692900	-3.34993000
H	-0.49496900	-3.30750900	-1.26565000
H	-2.85555900	-2.16703900	-1.14172000
H	-1.44705900	-2.46645900	1.17314000
H	-0.05645900	-2.72040900	3.14106000
H	-2.36348900	-1.58621900	3.25986000
C	0.81390000	1.41654100	0.25481000
N	0.50847000	2.58968100	-0.21532000
C	-0.79303000	3.30202100	-0.18819000
C	-1.60409000	2.84959100	1.02054000
H	-1.16471000	3.25880100	1.93422000
H	-2.62137000	3.23061100	0.92776000
H	-1.63616000	1.76148100	1.11523000
C	-1.47674000	2.98667100	-1.52133000
H	-2.48426000	3.40471100	-1.53091000
H	-0.91475000	3.42751100	-2.34901000
H	-1.53298000	1.90977100	-1.67095000
C	-0.47438000	4.79354100	-0.09204000
H	0.05691000	5.02148100	0.83321000

H	0.12737000	5.12862100	-0.94153000
H	-1.40819000	5.35635100	-0.10339000
C	2.16732000	0.91506100	0.00240000
C	2.85689100	0.28881200	1.04271000
C	2.77743000	1.08951200	-1.24397000
C	4.16303100	-0.13790800	0.84016000
H	2.35432100	0.12440100	1.98549000
C	4.07436000	0.63829200	-1.44648000
H	2.21202000	1.50267100	-2.07229000
C	4.76880100	0.03122200	-0.40230000
H	4.70143100	-0.62037800	1.64568000
H	4.53587000	0.74143200	-2.41977000
H	5.77844100	-0.32485800	-0.56286000
H	0.15696000	0.88977100	0.94416000
H	1.21147000	3.02718100	-0.79997000

cat3_am2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1127.920956	-1127.297385	-1127.269178	-1127.3551

C	-0.82456100	-2.37723900	-1.80917300
C	0.90099400	-0.74482600	2.62644500
C	-0.98604300	-2.68748800	-0.31897200
C	-0.04666200	-1.81978400	2.08528900
B	0.13972700	-2.02500100	0.54390700
C	-1.51569600	-1.63335600	2.48758200
C	-2.39209200	-2.42720600	0.23783900
C	-2.44381300	-2.61133500	1.75868100
C	1.55931200	-1.75901800	-0.10721100
C	2.80107500	-1.42370900	-2.12701600
C	3.62950300	-0.35329900	-1.43017700
C	3.66274300	-0.61557800	0.06965800
N	1.46833700	-1.47620700	-1.53990000
C	0.63875100	-2.46214200	-2.23026900
C	2.29875900	-0.90047400	2.03395600
H	-1.62871300	-1.73860200	3.57155300
H	-1.82232900	-0.61325400	2.23546000
H	-3.11896700	-3.08723800	-0.24682100
H	-2.68716400	-1.40107800	-0.00654900
H	-3.46932700	-2.47064100	2.10943800
H	2.70853300	-1.20150200	-3.19262000
H	4.64486500	-0.34144400	-1.83196400
H	3.17141900	0.62156900	-1.61323200
H	4.18474200	0.19247800	0.58898000
H	0.72848000	-2.26820200	-3.30174700
H	1.01883800	-3.48668600	-2.05553000
H	2.96986900	-0.15369800	2.46552300
H	2.71130200	-1.89392800	2.29170800

C	-0.23062700	1.59253600	-1.06456600
N	0.51427300	1.85575000	0.15697400
H	1.25674600	1.16648700	0.24767000
C	1.04929200	3.20605300	0.36295500
N	2.30099700	-0.69970800	0.58432900
C	1.69764600	3.20329500	1.74828200
H	2.49136000	2.45101800	1.79255000
H	2.13752600	4.17676900	1.97581400
H	0.95291600	2.96156300	2.50880700
C	2.11334600	3.58612200	-0.68017800
H	2.95493400	2.89004300	-0.62728900
H	1.70696700	3.55697900	-1.69318100
H	2.49402600	4.59479600	-0.50177400
C	-0.08910500	4.22712900	0.33983200
H	-0.58788800	4.25154900	-0.63138100
H	-0.83480300	3.98026400	1.09684100
H	0.30183200	5.22661300	0.54275600
C	-1.72578000	1.42030000	-0.84916700
C	-2.29679400	1.45392600	0.42052700
C	-2.55533500	1.18885400	-1.95024200
C	-3.66735700	1.25999000	0.58905700
H	-1.64377600	1.62864200	1.26590900
C	-3.92113200	0.98827400	-1.78613200
H	-2.12165900	1.16244100	-2.94543500
C	-4.48410800	1.02415300	-0.51160500
H	-4.09477700	1.28987800	1.58457600
H	-4.54774200	0.80628100	-2.65104700
H	-5.54795200	0.86957000	-0.38064700
H	-0.08350800	2.37421800	-1.82072400
H	0.15838400	0.66850100	-1.50552500
H	0.52253500	0.24325100	2.34821500
H	0.96157700	-0.78488800	3.71872700
H	-1.19202600	-1.36668400	-2.01080900
H	-1.41967700	-3.06434600	-2.41905100
H	-2.16111000	-3.64078500	2.01171300
H	-0.76397400	-3.76374000	-0.17922200
H	0.29018900	-2.79505900	2.48642000
H	3.30617400	-2.40343400	-2.02963000
H	2.12262500	-2.72802300	0.03026300
H	4.21176400	-1.55459000	0.26952500

cat3_im1d	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-857.486779	-856.975431	-856.952915	-857.025555

C	-0.07716800	-1.54183100	1.92640700
C	-2.42192000	1.00884000	-1.75090600
C	-1.46964000	-1.35891100	1.32594900
C	-2.72033700	-0.01123500	-0.65394800

B	-1.33809900	-0.29378500	0.11797500
C	-3.26970700	-1.35168300	-1.14063300
C	-2.07668800	-2.63813200	0.74737300
C	-3.40441000	-2.34621500	0.02616800
C	-0.69664100	1.10327000	0.62808000
C	1.39024300	1.99154600	1.67331500
C	1.46797300	3.00745600	0.54320600
C	0.07804200	3.28782600	-0.01939500
N	0.65600400	0.78013400	1.22530200
C	0.50928900	-0.19680700	2.35372800
C	-1.78831900	2.27154500	-1.15932000
H	-4.24113200	-1.24630400	-1.64172200
H	-2.57346800	-1.76811800	-1.87986800
H	-2.23959500	-3.40642200	1.51522200
H	-1.37014300	-3.05868700	0.02009200
H	-3.83788900	-3.28404500	-0.33491100
H	2.38223700	1.68236700	2.00836000
H	1.92669900	3.92237700	0.92329100
H	2.10192200	2.61104400	-0.25314100
H	0.15314100	3.97427700	-0.86590500
H	1.50077500	-0.30651800	2.79905600
H	-0.14293800	0.28617500	3.08657700
H	-1.59126200	3.00196700	-1.94918500
H	-2.50872700	2.73684500	-0.46172800
C	3.13852100	-1.32514300	-0.74869500
N	2.38157900	-0.30594000	-0.83177300
H	-0.51717400	-0.75792200	-0.69124000
H	1.22174500	0.33091000	0.46631700
N	-0.50970100	2.03708000	-0.46946800
H	-4.11348700	-1.93411500	0.75465800
H	-3.46327200	0.43237300	0.03058700
H	-2.13915000	-0.98516800	2.11855300
H	-1.24781200	1.58597100	1.46256800
H	-0.54787600	3.77499000	0.75210100
H	0.83781700	2.39703000	2.52538500
C	1.87087300	0.08785500	-2.14371900
H	1.09551300	0.83757000	-1.99438700
H	2.67776800	0.50874800	-2.75299100
H	1.43062300	-0.75591500	-2.68001200
C	3.65060600	-1.75239000	0.59848300
H	4.74315800	-1.77681800	0.59758500
H	3.30598100	-1.06796700	1.37145900
H	3.30249000	-2.76279800	0.82827500
C	3.55472000	-2.17227900	-1.92712800
H	2.68949300	-2.71838300	-2.31214800
H	3.93729500	-1.55263900	-2.73975600
H	4.31803300	-2.89395200	-1.64089100
H	-1.71991200	0.57108100	-2.46923100

H	-3.31642600	1.31447800	-2.30979400
H	0.58320500	-1.99060900	1.17519000
H	-0.05492400	-2.19408500	2.80954300

cat3_im1hts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-857.457261	-856.94913	-856.927902	-856.99516
Imaginary Frequency (one)		ν= 232.7i cm^{-1}		

C	-0.60792700	1.36551800	-2.05554400
C	-0.86827600	-2.49296200	1.25424200
C	-1.48576200	0.18923000	-1.64193200
C	-1.63166600	-1.80654200	0.12557100
B	-0.80947100	-0.52091700	-0.37008100
C	-3.06367100	-1.37440900	0.43848400
C	-2.93046300	0.54615500	-1.28909400
C	-3.70369700	-0.68489500	-0.78031900
C	0.74024100	-0.87810100	-0.65292600
C	2.88797600	0.03885500	-1.32184100
C	3.53438700	-0.67061700	-0.13970000
C	2.73474200	-1.91867100	0.21280800
N	1.48970900	0.35263200	-1.01626700
C	0.86018400	0.94871100	-2.21565800
C	0.58396000	-2.75673900	0.84080300
H	-3.69601700	-2.21624200	0.74940800
H	-3.04399400	-0.66658300	1.27927900
H	-3.47078800	0.98790900	-2.13677800
H	-2.91829800	1.30580400	-0.49406600
H	-4.73355900	-0.39866500	-0.54547700
H	3.41782300	0.96579200	-1.56201800
H	4.56450100	-0.93701900	-0.38602600
H	3.55481200	-0.00049700	0.72496300
H	3.16175900	-2.41118400	1.09080200
H	1.47173600	1.80825900	-2.50958400
H	0.92195600	0.21791800	-3.03924300
H	1.11952000	-3.25803400	1.65251700
H	0.57999100	-3.45219900	-0.01929400
N	1.35393100	-1.55341900	0.49416100
N	0.86772300	2.17575200	0.92056000
C	-0.02912900	1.67066900	1.73327700
H	-0.86263100	0.36864200	0.59331300
H	-3.76178900	-1.41569400	-1.59588600
H	-1.50318700	-0.53442600	-2.47383700
H	-1.67436900	-2.51643000	-0.71855100
H	0.81470800	-1.56383900	-1.53685100
H	2.93647400	-0.61458400	-2.20933100
H	2.78718400	-2.63341700	-0.63021300

H	1.39679900	1.44402700	0.35380700
C	0.75939200	3.48226300	0.28960900
H	1.07964300	4.25713900	0.98849500
H	1.42200700	3.49435700	-0.57316600
H	-0.25013400	3.71075700	-0.04910700
C	-1.23607600	2.47248900	2.11614100
H	-1.72362300	2.90685800	1.24565100
H	-1.94651400	1.83517500	2.63642200
H	-0.93025300	3.28196100	2.78742900
C	0.39719600	0.57011700	2.64997100
H	0.93729000	1.04874300	3.47582000
H	-0.47191300	0.05308600	3.04784500
H	1.04216800	-0.14307900	2.13318900
H	-0.68841000	2.14092000	-1.29024800
H	-0.92155500	1.82681300	-3.00122400
H	-0.87756000	-1.86467000	2.14922100
H	-1.31443100	-3.45419300	1.54060800

cat3_am1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-857.457261	-856.94913	-856.927902	-856.99516

C	-0.88286100	-1.09090700	-2.39071600
C	-0.57610800	-0.39002900	2.61700400
C	-1.68324700	-1.37349900	-1.11562600
C	-1.52170200	-0.99669200	1.57558400
B	-0.82596900	-1.18987100	0.18566500
C	-2.87014300	-0.27409900	1.45569400
C	-3.03789900	-0.65434300	-1.04746300
C	-3.72029800	-0.83630900	0.31209200
C	0.74355600	-1.39521600	0.11608200
C	2.69730000	-1.30496100	-1.27180900
C	3.45549300	-0.61953800	-0.14370500
C	2.85058400	-1.01173400	1.19684200
N	1.27766900	-0.98658800	-1.18394200
C	0.54370900	-1.61780000	-2.27812500
C	0.82228100	-0.98832200	2.49889100
H	-3.41819500	-0.33150600	2.40138400
H	-2.67903500	0.78936000	1.26866800
H	-3.69341700	-1.00184500	-1.85236300
H	-2.87792600	0.41738600	-1.21822700
H	-4.69717400	-0.34670800	0.30083000
H	3.07198400	-0.97121000	-2.24234900
H	4.51095400	-0.89776100	-0.17781500
H	3.37726700	0.46370200	-0.26605900
H	3.33651400	-0.46991500	2.01144700
H	1.08674500	-1.40506000	-3.20174800
H	0.52925200	-2.71814800	-2.15879500
H	1.47217200	-0.56361000	3.26728400

H	0.78679200	-2.08043400	2.67172700
C	-0.24045300	2.27863900	-0.60702900
N	0.44532300	2.28512400	0.68489400
H	0.98378800	1.42580700	0.76715900
N	1.42921400	-0.68977500	1.20164800
H	-0.69349400	1.28201000	-0.68034100
H	-3.90400400	-1.90343000	0.48659900
H	-1.88355200	-2.46225700	-1.08694400
H	-1.72735400	-2.04300800	1.87386600
H	2.85529900	-2.39863100	-1.20796200
H	0.91933500	-2.50227100	0.24657700
H	3.00458200	-2.09306200	1.37122500
C	1.29797100	3.43394500	0.94549200
H	1.73426200	3.32513000	1.93961900
H	2.12148200	3.57258300	0.23067800
H	0.70526900	4.35093200	0.95190400
C	-1.37456500	3.30166900	-0.62480900
H	-1.97755400	3.18855300	-1.52848000
H	-2.01282400	3.17151300	0.24998700
H	-0.98467800	4.32234400	-0.61716500
C	0.67630800	2.45382600	-1.82251000
H	1.46336100	1.69790600	-1.80754800
H	0.10848500	2.33893000	-2.74943300
H	1.12745200	3.44874700	-1.83599600
H	-0.83473000	-0.01149900	-2.56102300
H	-1.36884600	-1.53406900	-3.26556300
H	-0.95714000	-0.54732200	3.63094600
H	-0.50023300	0.68709200	2.44605500

cat4	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1040.799133	-1040.470943	-1040.453825	-1040.513407

C	-2.48455900	-0.47293100	0.04320900
C	2.48455300	-0.47296800	0.04320900
C	-1.35215900	-1.32951800	-0.46553700
C	1.35214100	-1.32953800	-0.46553900
B	-0.00000300	-0.53728400	-0.41836900
C	1.27088900	-2.72409300	0.17221000
C	-1.27093400	-2.72407800	0.17220100
C	-0.00002500	-3.46003300	-0.26401800
C	0.00000700	1.03725200	-0.52302900
C	-1.24592700	3.05265300	-0.12901000
C	0.00002800	3.69014800	0.46995100
N	1.20032300	1.61159300	0.07895300
C	1.24597300	3.05263400	-0.12901000
N	-1.20029900	1.61161100	0.07895400
C	-2.40646000	0.97222000	-0.40984200

C	2.40647500	0.97218400	-0.40984300
H	2.16078900	-3.30227500	-0.08428900
H	1.26563300	-2.60914100	1.25870100
H	-2.16083900	-3.30224600	-0.08431300
H	-1.26568900	-2.60913400	1.25869200
H	-0.00002200	-3.57975500	-1.35401300
H	-0.00003300	-4.46552200	0.16176800
H	-2.14549400	3.44628900	0.34879000
H	0.00003600	4.76517800	0.27975900
H	0.00002600	3.52069000	1.54759500
H	2.14554500	3.44625700	0.34879200
H	-3.27401900	1.48797900	0.00461700
H	-2.49292300	0.99216600	-1.51115600
H	3.27404200	1.48793100	0.00461500
H	2.49293700	0.99212800	-1.51115800
H	-1.30316500	3.29180500	-1.20805500
H	1.30321600	3.29178700	-1.20805500
H	-1.53306200	-1.44395700	-1.54791700
H	1.53304900	-1.44399100	-1.54791600
H	0.00000900	1.26608800	-1.63122300
F	-2.49793500	-0.50311500	1.41067500
F	-3.69529200	-0.97972300	-0.36447700
F	3.69527900	-0.97977700	-0.36447700
F	2.49792800	-0.50315000	1.41067400

cat4_bts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1041.948879	-1041.603506	-1041.586511	-1041.645361
Imaginary Frequency (one)		ν= 1206.5i cm^{-1}		

C	-2.57828700	-0.04039300	-0.07274000
C	2.38153200	-0.90515900	0.00317400
C	-1.56818000	-1.07658300	-0.49296400
C	1.08201800	-1.55544800	-0.37691900
B	-0.09983100	-0.50479600	-0.19707800
C	0.76450100	-2.87561400	0.32755700
C	-1.75634400	-2.43650900	0.19527700
C	-0.60476500	-3.39827300	-0.13155200
C	0.20251200	1.00655500	-0.67196000
C	-0.64582200	3.17998300	0.20039200
C	0.77985600	3.53773400	0.59661800
N	1.50176200	1.38140900	-0.15538400
C	1.77681100	2.79906600	-0.29072400
N	-0.83454000	1.72016100	0.12426800
C	-2.17841300	1.39587500	-0.39112100
C	2.55925600	0.48666300	-0.59194100
H	1.53992400	-3.61960400	0.12825400

H	0.74658000	-2.70714100	1.40847400
H	-2.71349000	-2.88449100	-0.08528000
H	-1.78273800	-2.27578400	1.27654100
H	-0.57541500	-3.57601200	-1.21314300
H	-0.80289800	-4.36416100	0.33897000
H	-1.36647200	3.57791800	0.91649000
H	0.90809400	4.61898800	0.51694300
H	0.95789100	3.23988400	1.63126100
H	2.79596500	2.99877800	0.04441700
H	-2.90801500	2.05073700	0.08540900
H	-2.21753800	1.54929100	-1.47467000
H	3.51560800	0.87037600	-0.23414000
H	2.62047000	0.38138000	-1.68680600
H	-0.87435100	3.60623000	-0.78673500
H	1.68924300	3.14334300	-1.33689500
H	-1.68101500	-1.19335600	-1.57833900
H	1.15270400	-1.74446900	-1.45842100
H	0.07613100	1.25199400	-1.74380600
H	-0.15659600	-0.19057200	1.18338100
H	-0.51369200	0.70237700	1.04243700
F	-2.78671600	-0.09809100	1.28608100
F	-3.80822300	-0.24436600	-0.64916700
F	2.48239700	-0.81150700	1.36667400
F	3.46033700	-1.66049100	-0.40244700

cat4_c	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1041.993455	-1041.640874	-1041.62371	-1041.682849

C	-2.48898900	-0.55576700	0.00671300
C	2.50667700	-0.46470000	0.05866400
C	-1.31358500	-1.35298800	-0.45674300
C	1.36672900	-1.31280000	-0.41964100
B	0.01612600	-0.56002400	0.02934900
C	1.33566600	-2.74321300	0.12149900
C	-1.24507700	-2.78173200	0.09109000
C	0.06133700	-3.46407700	-0.35024900
C	0.03086300	0.97692300	-0.48576800
C	-1.29294000	3.07771200	-0.07122900
C	0.00405200	3.74711300	0.35827500
N	1.18939400	1.66846400	0.03205200
C	1.20099800	3.07973900	-0.31348500
N	-1.21087300	1.60174600	0.13098000
C	-2.43230800	0.92001700	-0.39174000
C	2.41698400	0.99260200	-0.38854700
H	2.21702500	-3.31184900	-0.19045400
H	1.34326400	-2.70103700	1.21441800

H	-2.10189900	-3.38045800	-0.23361400
H	-1.27263300	-2.73530100	1.18354200
H	0.07447100	-3.52383700	-1.44553100
H	0.06868900	-4.49340800	0.01763000
H	-2.15725200	3.45058000	0.47997400
H	-0.05277100	4.80561700	0.09886200
H	0.12137500	3.66778600	1.44127100
H	2.12540600	3.52946200	0.05267000
H	-3.30975000	1.42488200	0.01161700
H	-2.41715700	1.00984300	-1.47733000
H	3.26850300	1.51827100	0.04645900
H	2.53180900	1.00278200	-1.48448900
H	-1.46687800	3.22024600	-1.14025900
H	1.15881500	3.23709600	-1.40700200
H	-1.38212800	-1.38274500	-1.55371300
H	1.45157900	-1.34268300	-1.51571700
H	-0.10246500	1.14728800	-1.57358800
H	-0.01386200	-0.46711500	1.25272300
H	-1.11970700	1.37333000	1.12788000
F	-2.61305400	-0.57155800	1.37731900
F	-3.69862700	-1.00232500	-0.47862700
F	2.60509100	-0.49155800	1.42432500
F	3.72912900	-0.91823300	-0.40594500

cat4_im2d	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1525.017773	-1524.424863	-1524.394336	-1524.483293

C	-0.29190400	2.50813600	0.41804100
C	-3.51646100	-1.12029700	-0.77360000
C	-1.75796500	2.25878100	0.27942900
C	-3.48634200	0.32004200	-0.36064700
B	-1.93700500	0.69865700	-0.12846200
C	-4.26969800	0.65933400	0.90868900
C	-2.59425500	2.52431800	1.53363000
C	-4.06305700	2.13613600	1.28769300
C	-1.05729500	0.30200300	-1.42693300
C	1.33222100	0.17823500	-2.14491000
C	1.10392900	-1.28745000	-2.47846300
C	-0.35946000	-1.53489500	-2.83372000
N	0.38724200	0.59807400	-1.06849900
C	0.52009300	2.05797700	-0.79517700
C	-2.59858600	-1.44249400	-1.95042100
H	-5.33905800	0.45745200	0.79123300
H	-3.90452800	0.02389900	1.72067500
H	-2.53834800	3.57239900	1.84524800
H	-2.19481300	1.91786400	2.35204300

H	-4.64919600	2.36733800	2.18114100
H	2.34910600	0.37371400	-1.80523900
H	1.75534800	-1.56146900	-3.31019600
H	1.37293500	-1.89802300	-1.61377900
H	-0.52443700	-2.59961500	-3.01087900
H	1.57147400	2.28351200	-0.63237200
H	0.16372800	2.58759600	-1.67888100
H	-2.67451600	-2.51503400	-2.13796400
H	-3.00442700	-0.91276700	-2.82833500
C	2.93748800	-1.42412800	1.04751900
N	1.68469200	-1.27673500	1.18265700
H	-1.48915600	0.01245800	0.77915400
H	0.60685000	0.06773700	-0.20115400
C	0.90215300	-2.24577700	1.97509500
N	-1.19432900	-1.10782500	-1.72287300
C	1.72664900	-3.33790900	2.65902100
H	2.47733200	-2.92002400	3.33427900
H	1.05175100	-3.95682400	3.25150200
H	2.22159200	-3.99169100	1.93630200
C	-0.11925000	-2.88864600	1.03498500
H	-0.77707600	-3.54745800	1.60554600
H	-0.73040800	-2.13911400	0.53672800
H	0.39246400	-3.48847200	0.27617600
C	0.18557000	-1.40274700	3.03659500
H	0.90997600	-0.98128000	3.73741500
H	-0.35830200	-0.58729800	2.56126200
H	-0.51768300	-2.02627500	3.59189000
C	3.75564300	-0.39209900	0.37248000
C	3.47869800	0.96096000	0.58828700
C	4.81307100	-0.75821000	-0.46235900
C	4.24094400	1.93569300	-0.04848000
H	2.66576200	1.22925900	1.25328600
C	5.55921800	0.21829100	-1.11455800
H	5.03992100	-1.80803500	-0.61079300
C	5.27326600	1.56594000	-0.90878500
H	4.03475400	2.98385100	0.13283600
H	6.36743400	-0.07022700	-1.77459200
H	5.86352700	2.32625000	-1.40455200
H	3.48028400	-2.29177600	1.43002500
H	-4.46110000	2.76533600	0.48201800
H	-3.90430100	0.88353400	-1.20773900
H	-2.09503100	2.92007300	-0.53200100
H	-1.22837300	0.91932500	-2.33439500
H	-0.61560300	-0.99475800	-3.76458300
H	1.10926100	0.81319600	-3.00648800
F	0.24030100	1.86265100	1.51517200
F	0.03443300	3.83819500	0.58703700
F	-3.18159500	-1.94324800	0.27418900

F	-4.77907000	-1.52978600	-1.16550500

cat4_im2ets	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1524.997586	-1524.409834	-1524.380083	-1524.46669
Imaginary Frequency (one)		ν= 737.3i cm^{-1}		

C	0.04681700	2.34675500	-0.01542000
C	-3.66137000	-0.94641400	-0.57333500
C	-1.44089000	2.27580400	-0.09805700
C	-3.41889000	0.52231700	-0.41661200
B	-1.82959200	0.70237700	-0.19572200
C	-4.15294300	1.20137000	0.74074200
C	-2.22364400	2.90045900	1.05716000
C	-3.73367400	2.67866600	0.85111700
C	-0.99116100	-0.05303700	-1.34976900
C	1.26629000	-0.55985100	-2.11138600
C	0.87984200	-2.03071500	-2.19320800
C	-0.61666200	-2.16542500	-2.45306800
N	0.47228200	0.11056800	-1.05974600
C	0.74230800	1.56137000	-1.12008300
C	-2.79041200	-1.59846200	-1.64275900
H	-5.24036400	1.13970900	0.62725100
H	-3.89241500	0.68173200	1.66766400
H	-2.02224600	3.97236700	1.15827400
H	-1.91389300	2.42119600	1.99127000
H	-4.28252300	3.15193200	1.67021100
H	2.32942700	-0.43104900	-1.89824500
H	1.44782800	-2.51057600	-2.99295100
H	1.12639100	-2.53215000	-1.25347800
H	-0.91057100	-3.21827800	-2.45085100
H	1.81422200	1.73290100	-1.06303100
H	0.38744300	1.95731900	-2.07893700
H	-3.04377800	-2.66057100	-1.66723500
H	-3.08889400	-1.15522500	-2.60855700
C	2.70768200	-1.17547900	1.16332600
N	1.43598300	-1.06461000	1.16484700
H	-1.53168600	0.16892300	0.86082500
H	0.89807700	-0.45153700	0.24917300
C	0.61705000	-1.76337000	2.20918400
N	-1.35419600	-1.46204400	-1.41638400
C	1.44533600	-2.71940300	3.06812700
H	2.21131000	-2.20915800	3.65684700
H	0.75840700	-3.19033900	3.77106500
H	1.90416300	-3.51539400	2.47607900
C	-0.49306300	-2.54913300	1.51910300
H	-1.14624600	-2.97243100	2.28385700
H	-1.08853500	-1.92465200	0.86038100

H	-0.06850500	-3.37076700	0.93551400
C	0.05488400	-0.65142500	3.10285000
H	0.86939300	-0.12779000	3.60885800
H	-0.52107400	0.06161000	2.51922100
H	-0.59366800	-1.10447200	3.85459000
C	3.63554000	-0.35864800	0.36464500
C	3.55531600	1.03375100	0.42353700
C	4.66866400	-0.97724300	-0.34738600
C	4.48655700	1.80418800	-0.26727800
H	2.76665500	1.49998300	1.00117100
C	5.57706400	-0.20236000	-1.05532900
H	4.74411900	-2.05849500	-0.36118300
C	5.48552000	1.18875100	-1.01458500
H	4.42448200	2.88400800	-0.22196700
H	6.36211600	-0.67865400	-1.62820600
H	6.20309600	1.79132300	-1.55667700
H	3.17190200	-1.89088100	1.83555900
H	-4.03685100	3.19669900	-0.06708200
H	-3.73254000	0.97921700	-1.36663700
H	-1.70257600	2.79094500	-1.03387500
H	-0.84881000	-1.75428500	-3.45437400
H	-1.13496700	0.40283400	-2.36032900
H	1.05200300	-0.07181700	-3.07261700
F	0.51528300	1.86265800	1.20202100
F	0.55083300	3.63240800	-0.08908200
F	-3.46083500	-1.61301300	0.61520900
F	-4.96954500	-1.23519200	-0.92627100

cat4_im2f	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1525.003163	-1524.411897	-1524.381471	-1524.470103

C	-0.07633000	2.45801800	0.23343200
C	-3.48791700	-1.03497000	-0.78877900
F	0.45135700	1.82208200	1.36149500
F	0.31242600	3.77630500	0.38158700
F	-4.76197400	-1.37887700	-1.21187100
F	-3.25978500	-1.83589500	0.31168800
C	-1.55273800	2.27038200	0.14728400
C	-3.37080700	0.41355100	-0.43091300
B	-1.79961800	0.70257100	-0.18814600
C	-4.15487100	0.85618700	0.80592300
C	-2.37568100	2.64772400	1.37855800
C	-3.86256200	2.33195800	1.13189200
C	-0.90470200	0.19439600	-1.43044500
C	1.36601000	0.01520600	-2.24572400
C	1.14511600	-1.47529700	-2.47190300
C	-0.33088200	-1.75009700	-2.73963700
N	0.52508600	0.46964100	-1.13370400

C	0.65832100	1.92091400	-0.98764100
C	-2.54735100	-1.47351300	-1.90718400
H	-5.23392400	0.71852300	0.67841200
H	-3.84616200	0.23322900	1.65114100
H	-2.26523900	3.70593000	1.63948800
H	-2.02157000	2.06383900	2.23475000
H	-4.44649500	2.63326000	2.00638600
H	2.41513100	0.22980200	-2.02399700
H	1.75136300	-1.81767900	-3.31354500
H	1.45430400	-2.02881000	-1.58001700
H	-0.50956700	-2.82414100	-2.84368100
H	1.71207300	2.18692100	-0.90795100
H	0.25201100	2.44298400	-1.86751200
H	-2.70436100	-2.54350900	-2.06278100
H	-2.87688200	-0.94741500	-2.82006200
C	2.66439200	-1.33583900	1.15247000
N	1.39980500	-1.17388000	1.26095800
H	-1.43877000	0.04381000	0.78007600
H	0.93370400	-0.45743900	0.64058100
C	0.52356900	-1.98593200	2.16277300
N	-1.13171400	-1.23564000	-1.63909600
C	1.34176300	-2.97641900	2.98499000
H	2.08238100	-2.48266600	3.61915100
H	0.64388600	-3.49882300	3.63888800
H	1.82863000	-3.73253800	2.36448200
C	-0.47710300	-2.73094300	1.28310600
H	-1.23267900	-3.19072400	1.92135100
H	-0.97175700	-2.06577400	0.57899400
H	0.03613800	-3.51660800	0.72193600
C	-0.15375100	-0.98079700	3.10012400
H	0.59070600	-0.48456600	3.72659500
H	-0.70749100	-0.23500900	2.53369500
H	-0.84903000	-1.52380200	3.74178700
C	3.56824300	-0.45021700	0.42683300
C	3.40520000	0.93574600	0.49260600
C	4.65262800	-1.00941000	-0.25930300
C	4.31734000	1.75787400	-0.15924500
H	2.57900900	1.35673900	1.05155800
C	5.53827100	-0.18188200	-0.93353500
H	4.78424700	-2.08505300	-0.28025600
C	5.37016800	1.20177600	-0.88040900
H	4.20026600	2.83269200	-0.10509200
H	6.36393500	-0.60921100	-1.48708000
H	6.07183400	1.84776000	-1.39263100
H	3.10517600	-2.18326200	1.66486000
H	-4.21220000	2.95049900	0.29608100
H	-3.72888000	0.96807400	-1.31052500
H	-1.87143200	2.89166500	-0.70226300

H	-1.13856700	0.73088800	-2.38697300
H	-0.61773600	-1.26928400	-3.69455400
H	1.09762900	0.56294800	-3.16537300

cat4_im2gts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1524.989562	-1524.402944	-1524.373425	-1524.45819
Imaginary Frequency (one)		ν= 153.1i cm^{-1}		

C	0.25421200	-2.34612100	-1.74894700
C	0.40803900	-0.02817700	2.69141900
C	-0.24508100	-2.49870000	-0.33771700
C	-0.17493300	-1.24931800	2.03622200
B	0.28179000	-1.20954800	0.48770200
C	-1.68048800	-1.51375500	2.18033000
C	-1.74801600	-2.73421000	-0.12388100
C	-2.08640400	-2.77566600	1.38431500
C	1.88261800	-1.07542900	0.35887700
C	3.75141100	-0.94271900	-1.19358500
C	4.33584800	0.20857500	-0.37323300
C	3.85568100	0.14648200	1.07802600
N	2.29197800	-0.98636300	-1.05964800
C	1.76852700	-2.11619800	-1.83749800
C	1.92890600	0.07297500	2.51119400
H	-1.96778900	-1.64237700	3.23279700
H	-2.24827600	-0.65562900	1.80621500
H	-2.08085100	-3.66898200	-0.59507600
H	-2.32073000	-1.92870200	-0.59497700
H	-3.16272800	-2.95095500	1.50802500
H	4.01198200	-0.82794400	-2.25340300
H	5.43066300	0.16205800	-0.40371800
H	4.03410000	1.16406600	-0.81434100
H	4.19420000	1.03282000	1.62986800
H	2.02006500	-1.96525900	-2.89304300
H	2.23444300	-3.07119500	-1.52754700
H	2.26161800	0.99596800	2.99947700
H	2.35996900	-0.76953400	3.08471800
N	2.39389900	0.08189800	1.12071700
H	-0.25943900	-0.18628600	-0.07048300
H	-1.58415800	-3.64660500	1.83142200
H	0.29238000	-3.38062300	0.04964100
H	0.35659500	-2.09271600	2.50839500
H	2.35316900	-2.00276000	0.79151700
H	4.20515100	-1.89655400	-0.85230900
H	4.30625800	-0.73646000	1.57696900
C	-0.97917800	1.32622400	-0.92717300
N	-0.41329000	2.44128900	-0.52867000

C	0.83262000	3.09850300	-1.01599400
C	0.40388300	4.47900900	-1.55139500
H	-0.08367300	5.07674100	-0.77277800
H	1.28513800	5.03175100	-1.88934000
H	-0.28640900	4.38121500	-2.39478500
C	1.47481600	2.26397300	-2.12637900
H	2.40593100	2.75101100	-2.42960300
H	1.70927600	1.24652000	-1.79295900
H	0.83176400	2.21518600	-3.01231900
C	1.77154800	3.25410700	0.18956500
H	1.29763000	3.84909200	0.97926100
H	2.02571600	2.26783900	0.58763500
H	2.68229300	3.77705400	-0.11873500
C	-2.39078800	1.06090900	-0.60932100
C	-3.15580700	0.38188900	-1.56992400
C	-3.00924200	1.54138100	0.55650200
C	-4.52821500	0.22268400	-1.38587400
H	-2.66602800	-0.02990700	-2.44618800
C	-4.37801500	1.37094400	0.73830000
H	-2.41209300	1.98250600	1.34894000
C	-5.14187400	0.72179100	-0.23646700
H	-5.11445100	-0.29909500	-2.13567500
H	-4.84836100	1.73052400	1.64809600
H	-6.20995800	0.59233900	-0.09047100
H	-0.54424400	0.81316800	-1.77386500
H	-0.86817900	2.93691000	0.23038400
F	-0.18237400	1.14512900	2.20103400
F	0.17166000	0.02283900	4.05908900
F	-0.40001000	-1.29252600	-2.41008800
F	-0.01799300	-3.45101300	-2.54350400

cat4_am2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1525.02879	-1524.436889	-1524.405711	-1524.497604

C	-1.82663200	-1.97652600	-1.48443300
C	1.03236700	-0.92076800	2.52717700
C	-1.87625300	-1.96638100	0.02362900
C	-0.34233700	-1.43898400	2.17626600
B	-0.45594600	-1.78432900	0.65413500
C	-1.50568800	-0.58914500	2.71056600
C	-2.92887100	-1.03252700	0.64068600
C	-2.85656100	-1.07620300	2.17189200
C	0.83847300	-2.16316000	-0.16929700
C	1.78885100	-2.36788300	-2.36787400
C	3.01596400	-1.60470100	-1.89244500
C	3.21055700	-1.81255900	-0.39701500
N	0.62628700	-1.94034200	-1.59763700

C	-0.57561300	-2.61794300	-2.05416700
C	2.16162000	-1.57415200	1.74961900
H	-1.50130500	-0.59837000	3.80279100
H	-1.35423500	0.44230200	2.39145000
H	-3.92495200	-1.31867200	0.29608500
H	-2.74746500	-0.01132500	0.29768700
H	-3.64833100	-0.44701400	2.58402100
H	1.59949800	-2.17029000	-3.42463300
H	3.90213600	-1.93868100	-2.43504700
H	2.86383900	-0.54163900	-2.08866800
H	4.04446600	-1.20993300	-0.02997400
H	-0.63836700	-2.53830000	-3.14034500
H	-0.58593300	-3.68932100	-1.78879900
H	3.08756900	-1.08664600	2.05873200
H	2.21578900	-2.63434800	2.05010300
C	0.19232700	1.71745300	-1.36315200
N	1.27532300	1.68776300	-0.40262000
H	1.64082500	0.75214700	-0.27370300
C	2.33966100	2.68553300	-0.47824200
N	1.99878900	-1.41210400	0.31331600
C	3.26872100	2.40972200	0.70495300
H	3.70012300	1.40718400	0.61843200
H	4.08796400	3.13118400	0.73403700
H	2.70803600	2.45554600	1.63878100
C	3.15308400	2.60679200	-1.78212300
H	3.64486000	1.63392500	-1.86255300
H	2.51460600	2.74286400	-2.65766500
H	3.92536400	3.37987800	-1.80921400
C	1.74025100	4.08633300	-0.33569100
H	1.03949900	4.30377000	-1.14479500
H	1.20308700	4.17183500	0.60950600
H	2.53162200	4.83884400	-0.36315100
C	-1.13236000	2.18150500	-0.77109400
C	-1.26630400	2.44979000	0.58910400
C	-2.25580100	2.29918500	-1.59312000
C	-2.49979300	2.82803200	1.11975500
H	-0.38881900	2.33869600	1.21401400
C	-3.48687300	2.67192300	-1.06730900
H	-2.16568600	2.07524200	-2.65090500
C	-3.61426300	2.93881500	0.29545700
H	-2.58752000	3.03409700	2.18050600
H	-4.34929000	2.75149900	-1.71815500
H	-4.57305700	3.23037400	0.70634900
H	0.42272600	2.35096300	-2.22907600
H	0.03926300	0.70890500	-1.75751300
H	-3.04850100	-2.09830700	2.52071700
H	-2.12296300	-3.00538800	0.30613700
H	-0.39536300	-2.44195400	2.63653400

H	1.95600200	-3.45461800	-2.24893000
H	1.02269200	-3.26230600	0.00546200
H	3.44396500	-2.87402100	-0.19567000
F	1.08727100	0.42983100	2.32051700
F	1.29087900	-1.11204000	3.86426000
F	-1.91609100	-0.69823600	-1.96614100
F	-2.91010000	-2.64828900	-1.99791000

cat4_im1d	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1254.608046	-1254.12795	-1254.102628	-1254.180293

C	0.95306200	1.95234300	-1.11827100
C	-2.79670500	-0.83754400	0.62896800
C	-0.51211300	2.03074100	-0.83838400
C	-2.51980200	0.54239300	0.11710200
B	-0.94198500	0.59753200	-0.21298600
C	-2.86468000	1.69005200	1.06637500
C	-0.92861900	3.12998300	0.14271800
C	-2.43272000	3.03333600	0.45278300
C	-0.53213600	-0.62519700	-1.19237900
C	1.51098100	-1.69878600	-2.14180700
C	1.02783700	-3.02015900	-1.56142900
C	-0.49223700	-3.02647100	-1.43440700
N	0.97016000	-0.56775000	-1.34059200
C	1.36331700	0.73329500	-1.94563600
C	-2.32767500	-1.93986400	-0.31635200
H	-3.93443400	1.71936700	1.29646200
H	-2.33150500	1.53375800	2.00876200
H	-0.69602000	4.12816200	-0.24255500
H	-0.36430000	2.99711600	1.07024900
H	-2.71325000	3.84830800	1.12562100
H	2.60032200	-1.62839800	-2.13535200
H	1.36573000	-3.83189900	-2.20808600
H	1.46899400	-3.15791000	-0.57241200
H	-0.82062800	-3.95390400	-0.96071700
H	2.44627900	0.74646500	-2.07015700
H	0.88709400	0.80193100	-2.92474800
H	-2.56271100	-2.89662700	0.15358300
H	-2.93068100	-1.85358300	-1.23528500
C	3.10666200	-0.37345900	1.63625200
N	2.09860400	-1.01635300	1.19849600
H	-0.30588000	0.43146400	0.81748800
H	1.38487800	-0.65568500	-0.36105900
N	-0.89603500	-1.90164900	-0.60620500
H	-2.99301400	3.19013000	-0.47722500
H	-3.11502300	0.64377400	-0.80248000
H	-0.99479100	2.20345500	-1.81122600
H	-0.91112500	-0.54660600	-2.23428600

H	-0.95628900	-2.97777700	-2.43711500
H	1.15135900	-1.56486200	-3.16581800
F	1.69495800	1.92420200	0.04249400
F	1.44194000	3.03111700	-1.82973800
F	-2.21285900	-1.04191600	1.85659000
F	-4.14705800	-1.06732400	0.82924900
C	1.12677400	-1.54380700	2.15656300
H	0.25725500	-1.89769100	1.60829300
H	1.56814600	-2.36865300	2.72554900
H	0.78801100	-0.77604700	2.85518200
C	4.10582400	0.18751800	0.66511200
H	4.08148700	1.27829700	0.69949200
H	5.11382500	-0.13730700	0.93201100
H	3.88121900	-0.14167800	-0.34799700
C	3.36266300	-0.10616300	3.09856900
H	2.59480800	0.56897600	3.48477800
H	3.30855200	-1.02827100	3.67978100
H	4.33710600	0.35431800	3.25029100

cat4_im1ets	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1254.603542	-1254.12762	-1254.102958	-1254.178493
Imaginary Frequency (one)		ν= 1091.1i cm^{-1}		

C	0.93941900	2.00933900	-1.01333600
C	-2.78127400	-0.92601500	0.53109900
C	-0.53376600	2.04297400	-0.77250400
C	-2.52552100	0.47340000	0.06667400
B	-0.93555800	0.58436000	-0.18979400
C	-2.94967700	1.58827600	1.02275500
C	-1.02220400	3.10998000	0.20932000
C	-2.53392500	2.95807000	0.45734300
C	-0.42791700	-0.60280500	-1.16661500
C	1.62825500	-1.56810200	-2.10696900
C	1.19268500	-2.92998900	-1.58023600
C	-0.32689000	-2.99489100	-1.47039100
N	1.06189200	-0.49483300	-1.26612100
C	1.39436800	0.81937400	-1.85418500
C	-2.23124600	-1.98869900	-0.41494700
H	-4.02911000	1.58069000	1.20597000
H	-2.45404300	1.42870500	1.98511900
H	-0.81011600	4.12302400	-0.14878700
H	-0.48918900	2.97939400	1.15586400
H	-2.86893200	3.74872700	1.13456900
H	2.71831500	-1.47501900	-2.11266600
H	1.56174600	-3.70932100	-2.24969000
H	1.62774700	-3.09867500	-0.59189700
H	-0.63227600	-3.94771000	-1.03117500

H	2.47454600	0.89223100	-1.99375000
H	0.91799700	0.90444200	-2.83700600
H	-2.47111800	-2.96465500	0.01241800
H	-2.78181500	-1.88853600	-1.36515300
C	3.02268000	-0.35795400	1.59589100
N	1.91487400	-0.83851600	1.18279000
H	-0.35479900	0.44453500	0.87743200
H	1.52403100	-0.64840600	-0.00255100
N	-0.78739400	-1.90724400	-0.62102700
H	-3.05999900	3.11753700	-0.49197500
H	-3.07864200	0.57765000	-0.87841300
H	-0.99158300	2.21280500	-1.75781600
H	-0.77539500	-2.93085500	-2.47912800
H	-0.80717100	-0.52107000	-2.21257500
H	1.27004500	-1.43185400	-3.13596900
F	1.64934100	1.97346600	0.17455500
F	1.41926300	3.12600500	-1.67237500
F	-2.24618900	-1.14381700	1.78283800
F	-4.13039500	-1.20453100	0.66777800
C	3.98602200	0.26277100	0.63348900
H	4.98634700	-0.13483100	0.81436600
H	3.69974300	0.07350500	-0.39679900
H	4.01118400	1.34132900	0.79713200
C	0.96674500	-1.46010700	2.11001400
H	0.57121100	-0.71604600	2.80160000
H	0.13771200	-1.84810700	1.52554200
H	1.46024500	-2.25868000	2.66872000
C	3.41175200	-0.38038200	3.04641100
H	2.62019900	0.05787500	3.65623000
H	3.55495700	-1.40958600	3.38469500
H	4.33513100	0.17169900	3.20711600

cat4_im1f	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1254.606215	-1254.126981	-1254.10192	-1254.179185

C	0.82838500	2.16723900	-0.89082900
C	-2.68252100	-1.09658900	0.46174000
F	1.54008600	2.08491900	0.29714300
F	1.23509500	3.36409600	-1.45269500
F	-4.00975200	-1.48013700	0.54367200
F	-2.17757700	-1.33970500	1.72750200
C	-0.64199000	2.09074100	-0.64708100
C	-2.51599300	0.33985400	0.08236700
B	-0.93522100	0.57468800	-0.15648000
C	-3.02563900	1.36595400	1.09491500
C	-1.20324900	3.06214300	0.39239300
C	-2.70235600	2.79273400	0.61658800
C	-0.35190600	-0.50705800	-1.20857000

C	1.69594000	-1.24244400	-2.30275900
C	1.40197800	-2.67054400	-1.85934400
C	-0.09738100	-2.86328600	-1.65936000
N	1.11143800	-0.29166100	-1.34907300
C	1.34637000	1.07845400	-1.82577000
C	-2.03110500	-2.07038400	-0.51482500
H	-4.10346400	1.27283200	1.26477700
H	-2.52832200	1.18655100	2.05297000
H	-1.05962100	4.10698900	0.09694900
H	-0.66657500	2.91183800	1.33419100
H	-3.09573200	3.51526600	1.33726500
H	2.77461600	-1.06748000	-2.37050200
H	1.77630000	-3.37128300	-2.60837900
H	1.92245500	-2.87795100	-0.91979400
H	-0.30311100	-3.86341100	-1.26747400
H	2.41842900	1.23709400	-1.96787900
H	0.85648800	1.22964200	-2.79781400
H	-2.19430300	-3.07920400	-0.12838700
H	-2.58779500	-1.97848900	-1.46280600
C	2.95134800	-0.40338000	1.66913500
N	1.86968700	-0.92240300	1.22747200
H	-0.34728300	0.42254600	0.90994000
H	1.56354600	-0.66576700	0.20671300
N	-0.59822100	-1.86659700	-0.72159000
H	-3.23273600	2.97320200	-0.32654400
H	-3.06374700	0.46021300	-0.86383800
H	-1.11548300	2.28257300	-1.62077000
H	-0.79501900	-0.40138400	-2.23040700
H	-0.60891500	-2.77603700	-2.63599800
H	1.26592400	-1.07208000	-3.30235100
C	0.96496700	-1.77568600	1.99281100
H	0.88256200	-2.72701900	1.47098400
H	1.33647200	-1.92583500	3.00212700
H	-0.01975900	-1.31617400	1.99032700
C	3.81714000	0.40214000	0.75750300
H	4.84785700	0.05692800	0.85777700
H	3.49236700	0.32311600	-0.27490400
H	3.77280800	1.45024000	1.05711000
C	3.40534800	-0.57386800	3.09015600
H	2.62422500	-0.25732800	3.78198700
H	3.64007200	-1.62004700	3.29620000
H	4.29685200	0.02296700	3.26826200

cat4_im1gts	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1254.591058	-1254.111708	-1254.087584	-1254.160535
Imaginary Frequency (one)		ν= 114.9i cm^{-1}		

C	-2.01016900	0.96887500	-1.23473400
C	2.22246700	-1.55583200	-0.29737700
C	-1.27059700	-0.28405400	-1.57756400
C	0.95425800	-1.62078900	-1.08517500
B	0.04385100	-0.36612400	-0.64700100
C	0.13861400	-2.91125900	-1.01796300
C	-2.04351300	-1.60146200	-1.51221200
C	-1.12360900	-2.77789100	-1.89168800
C	0.87056400	1.01161200	-0.70615000
C	0.72661200	3.38928600	-0.30136600
C	2.00015200	3.30510700	0.53047500
C	2.86147600	2.14529600	0.04697700
N	0.00481700	2.11839000	-0.25960600
C	-1.13373700	2.21221300	-1.17229900
C	2.90959700	-0.19827400	-0.37292500
H	0.71892300	-3.77943900	-1.34564800
H	-0.15904800	-3.09733100	0.01929100
H	-2.92323400	-1.59785300	-2.16349100
H	-2.40074000	-1.75655500	-0.48816900
H	-1.69368500	-3.71026600	-1.85329400
H	0.07272600	4.18530500	0.06669800
H	2.55482000	4.24236500	0.44800800
H	1.74630100	3.15362300	1.58211900
H	3.75294200	2.04012200	0.67174200
H	-1.77159200	3.04561400	-0.86787100
H	-0.79987100	2.40692500	-2.20607600
H	3.81617800	-0.25620900	0.23411600
H	3.21728300	-0.06053700	-1.42467700
N	2.09131300	0.91091500	0.09975100
N	-1.93783800	0.16461100	2.39085300
C	-0.76495600	-0.41218500	2.42193300
H	-0.33822500	-0.55688200	0.56336400
H	-0.80926800	-2.64789700	-2.93387300
H	-0.92817600	-0.13111000	-2.61178400
H	1.26513700	-1.45917500	-2.12811400
H	1.17795100	1.23298000	-1.76615400
H	1.00018700	3.63866600	-1.34377800
H	3.19913100	2.35200000	-0.98681100
H	-1.93663200	1.13719900	2.11514200
C	-0.67598200	-1.88136000	2.68038000
H	0.29791500	-2.23613500	2.35942900
H	-0.78457400	-2.04347800	3.75857400
H	-1.45361900	-2.43532700	2.15926700

C	-3.21279700	-0.53434900	2.30081400
H	-3.32892500	-1.20498900	3.15040900
H	-4.00457500	0.20871100	2.31908300
H	-3.27894100	-1.08732600	1.36534700
C	0.42263300	0.44985000	2.68016100
H	0.50030800	0.57496900	3.76615200
H	1.31974700	-0.01439200	2.28557900
H	0.30238000	1.41370700	2.18838700
F	1.99746100	-1.85475300	1.04144600
F	3.14948900	-2.49291000	-0.70628200
F	-2.66509200	0.84130200	-0.01377200
F	-3.02454900	1.24938500	-2.12835700

cat4_am1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1254.61747	-1254.136318	-1254.110577	-1254.191312

C	-0.02593200	2.62932400	-0.32875600
C	-1.90483300	-1.98396900	-0.20720700
C	-1.36713400	1.95121500	-0.20413000
C	-2.38177200	-0.55341400	-0.13834300
B	-1.25895700	0.43726300	-0.59628800
C	-3.05149200	-0.16008500	1.18688200
C	-2.09641200	2.19838200	1.12456100
C	-3.36286200	1.34049700	1.22504800
C	-0.14114600	-0.04444200	-1.60456200
C	2.06364200	0.38823000	-2.48053500
C	2.41164000	-1.08307400	-2.29789600
C	1.14676900	-1.92617500	-2.37195900
N	1.06362900	0.77513000	-1.48939900
C	0.76587000	2.19382700	-1.54694600
C	-1.01662200	-2.27587400	-1.40097500
H	-3.96078300	-0.74664800	1.33296500
H	-2.37354500	-0.40707500	2.00742100
H	-2.33900000	3.25829300	1.22358500
H	-1.42479500	1.94575800	1.94862600
H	-3.88614900	1.57716600	2.15356400
H	2.95010700	1.00975900	-2.33732600
H	3.11147400	-1.39740600	-3.07479600
H	2.87837600	-1.21292500	-1.31933600
H	1.37361000	-2.97259400	-2.15891200
H	1.70282100	2.75277700	-1.54356600
H	0.19992000	2.48118200	-2.44957900
H	-0.72541500	-3.32523800	-1.33687100
H	-1.61812400	-2.14420600	-2.31788100
C	1.87869200	-1.23491300	1.84020700
N	2.68801600	-0.30095100	1.05175400
H	2.07342500	0.12511200	0.36384900

N	0.17872500	-1.45339800	-1.38699500
H	1.40915000	-1.89486100	1.10636700
H	-4.04511200	1.59519600	0.40514200
H	-1.98008700	2.36642800	-1.02303000
H	-3.12406000	-0.45995800	-0.95025200
H	1.68200900	0.56527300	-3.50295200
H	-0.57017400	0.08102200	-2.64132500
H	0.71746400	-1.87174700	-3.39043300
C	3.33839900	0.76064900	1.80783800
H	3.83998500	1.42789500	1.10440700
H	2.66088300	1.37278300	2.41702200
H	4.10569900	0.34402600	2.46339400
C	2.76042100	-2.08180300	2.75421800
H	2.17537600	-2.88049500	3.21409800
H	3.57713600	-2.52346400	2.18196700
H	3.18839000	-1.48123100	3.56047100
C	0.74890900	-0.56760300	2.63574000
H	0.18320200	0.10470600	1.98454800
H	0.06486600	-1.31712000	3.03700800
H	1.13724200	0.02116200	3.47006500
F	0.72226100	2.36735800	0.79137000
F	-0.17447000	3.99221600	-0.37758700
F	-2.97457400	-2.84451900	-0.25300400
F	-1.21749700	-2.29616500	0.93550600

cat3_Dimer1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1287.382167	-1286.661941	-1286.63263	-1286.71937

C	3.11184400	2.19202100	0.93049900
C	2.52804900	-2.64703200	-0.39564000
C	3.96258800	0.97105100	0.57109500
C	3.64850800	-1.63588900	-0.14073600
B	3.13329000	-0.35909900	0.60874600
C	4.48446700	-1.30180200	-1.38382500
C	4.76713600	1.12900400	-0.72610000
C	5.48046700	-0.16780800	-1.12075200
C	1.86513800	-0.46395400	1.55127900
C	0.13198200	0.73121200	2.69172400
C	-0.87606000	-0.32370500	2.26265200
C	-0.17691700	-1.65107200	2.01302600
N	1.19959800	0.83086800	1.70355300
C	2.14764600	1.87905700	2.06951000
C	1.58646900	-2.74345200	0.80074400
H	5.00788200	-2.19394400	-1.74212700
H	3.80755600	-0.99359400	-2.18989700
H	5.48744600	1.94774200	-0.63099600
H	4.08038400	1.41113700	-1.53394200

H	6.09180000	0.00164000	-2.01055200
H	-0.35103300	1.70713800	2.78573900
H	-1.64007400	-0.44682200	3.03395800
H	-1.38865100	-0.01018100	1.35214000
H	-0.88846800	-2.36211600	1.58618100
H	1.56788500	2.77183100	2.31568100
H	2.71564600	1.60201500	2.97816900
H	0.80583700	-3.48020600	0.59502700
H	2.14093800	-3.10107900	1.68953000
N	0.92280300	-1.47256800	1.07140000
H	2.52262600	2.49167000	0.05888200
H	3.74213800	3.04406800	1.20375700
H	2.93623900	-3.63644400	-0.62511500
H	1.94304100	-2.32792700	-1.26352900
H	0.55028700	0.46699100	3.68222200
H	0.19867000	-2.06391700	2.96880200
H	2.25706000	-0.78475400	2.56133400
H	4.68488500	0.81340500	1.39457000
H	6.16512000	-0.46487800	-0.31722400
H	4.33074200	-2.07651000	0.61141800
C	-0.94220300	-1.60259800	-1.88894800
C	-2.50840600	2.78025400	0.08625400
C	-0.86867900	-0.10008700	-2.17517200
C	-1.71525100	2.25851400	-1.11518800
B	-1.89505600	0.71281300	-1.31373500
C	-0.24122800	2.68441500	-1.11844600
C	0.55062200	0.48175700	-2.08365200
C	0.55085400	2.00597500	-2.24160100
C	-3.21776300	0.00878800	-0.79838100
C	-4.26122500	-2.06412200	-0.20009200
C	-4.87028300	-1.39260200	1.02207700
C	-5.04195300	0.09606400	0.75598200
N	-3.00191200	-1.41656100	-0.54143200
C	-2.38189600	-2.06447400	-1.69451000
C	-3.87759300	2.11564500	0.17508800
H	-0.15902300	3.77393500	-1.19599200
H	0.20019200	2.38787000	-0.16073300
H	1.20065200	0.01819500	-2.83482900
H	0.95435000	0.22683600	-1.09568500
H	1.57928200	2.37897300	-2.24460100
H	-4.07026300	-3.12170800	-0.00205200
H	-5.83391300	-1.84743700	1.26170200
H	-4.19701100	-1.52509600	1.87176500
H	-5.41436300	0.60513300	1.64833700
H	-2.40175300	-3.14213300	-1.51398600
H	-2.97086000	-1.88148000	-2.61421600
H	-4.43461500	2.52651300	1.02048800
H	-4.46443100	2.33906100	-0.73664600

N	-3.75970000	0.67694900	0.38531900
H	-0.39299500	-1.80007900	-0.96573200
H	-0.47381900	-2.18023700	-2.69341500
H	-2.62470400	3.86781000	0.03997100
H	-1.96287400	2.54937000	1.00650200
H	-4.97356400	-2.00379400	-1.04557500
H	-5.78686000	0.24161600	-0.05000700
H	-3.96453000	0.11066300	-1.64070100
H	-1.23972100	0.07292000	-3.20377500
H	0.11782400	2.27400600	-3.21349400
H	-2.18953100	2.66345900	-2.02960900

cat3_Dimer2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1287.354484	-1286.622618	-1286.596791	-1286.670574

C	-2.70900500	2.38845400	0.92284100
C	-0.54416200	-1.06803700	-2.28811800
C	-2.87665100	1.17932100	0.00995500
C	-1.76899700	-0.49584000	-1.58725800
B	-1.48522400	0.38963600	-0.23130700
C	-3.00935100	-1.38619300	-1.61498200
C	-4.10805000	0.27343600	0.14053600
C	-4.25944600	-0.61782000	-1.11773100
C	-0.39009900	1.45115600	-0.73566900
C	0.57160300	3.62488600	-0.55637800
C	1.96480500	3.04585400	-0.72621200
C	1.93918600	1.72453100	-1.48863700
N	-0.28389400	2.64434800	0.09359200
C	-1.59943000	3.26995100	0.32816200
C	0.62404500	-0.07828800	-2.30826900
H	-3.21237800	-1.69637200	-2.64819200
H	-2.84049000	-2.31685300	-1.07263600
H	-5.01866600	0.87992300	0.22399700
H	-4.08317100	-0.34038400	1.04265300
H	-5.09003900	-1.31517600	-0.97364300
H	0.61536400	4.53025600	0.05442600
H	2.58348100	3.73244700	-1.31016300
H	3.74624800	1.64711700	0.40343900
H	2.91624900	1.25123900	-1.49170900
H	-1.41685400	4.13554000	0.97084700
H	-1.98783300	3.66150600	-0.63122400
H	1.56028800	-0.56333400	-2.58629900
H	0.40152500	0.66964900	-3.07414400
N	0.92216800	0.70680600	-1.04002800
H	-2.49832600	2.12142600	1.96062100
H	-3.61752800	3.00306800	0.95001900
H	-0.76550700	-1.27157600	-3.34464300
H	-0.27347300	-2.00551800	-1.82926500

H	0.15345200	3.90752000	-1.54244400
H	1.68898000	1.97686800	-2.52301100
H	-0.70467900	1.80102600	-1.74109300
H	-3.01995200	1.64792500	-0.97753600
H	-4.56083800	0.04892600	-1.93370600
H	-2.07016800	0.34570800	-2.23003400
C	1.32750900	1.25730900	2.07899800
C	1.98692000	-2.78945600	-1.05879300
C	2.29423200	0.30707600	1.37968600
C	2.59029500	-1.59299600	-0.32790300
B	1.54550700	-0.45029300	0.16095400
C	3.97267400	-1.07738500	-0.73496400
C	3.72391200	0.79247600	1.07700200
C	4.59318100	-0.32726700	0.46322000
C	0.31942500	-1.26261400	0.87738700
C	-1.76789900	-1.00257800	2.11064900
C	-2.28528700	-2.29534500	1.51903600
C	-1.11656800	-3.17644500	1.10085400
N	-0.76432600	-0.29752400	1.25022000
C	-0.09444800	0.67170800	2.26243400
C	0.87063700	-3.37741100	-0.17999900
H	4.63473800	-1.91268500	-0.99455900
H	3.94049400	-0.44183500	-1.62647600
H	4.21088300	1.13514400	1.99844700
H	2.42857300	2.94843700	0.24897900
H	5.56710600	0.08638300	0.18618600
H	-2.56275100	-0.29781100	2.35090100
H	-2.86713700	-2.80418700	2.29231600
H	-2.94690000	-2.10797800	0.68424200
H	-1.48195400	-4.06168500	0.57389300
H	-0.79154600	1.48561900	2.41892800
H	-0.05200400	0.08570400	3.18050600
H	0.38857600	-4.21439600	-0.69342900
H	1.35490100	-3.79293800	0.72445900
N	-0.20305600	-2.45574500	0.22634600
H	1.23164200	2.20088100	1.56347100
H	1.66145300	1.48210900	3.10074000
H	2.73689700	-3.58126600	-1.17877500
H	1.62336500	-2.56369800	-2.06138800
H	-1.26069500	-1.26890800	3.04228400
H	-0.58477000	-3.52713200	2.00793900
H	0.73988700	-1.58999200	1.85518300
H	2.45607300	-0.51640800	2.08984300
H	4.78415000	-1.07527000	1.24126800
H	2.79149100	-2.03181900	0.66455900

cat3_im2_CP1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1126.701925	-1126.095013	-1126.070537	-1126.143906

C	0.03066500	-0.85512000	-2.42479500
C	3.29298900	1.05899500	1.10625700
C	1.45662900	-0.82241000	-1.89006800
C	2.98909500	0.00517200	0.03696500
B	1.43198300	-0.11634000	-0.42126300
C	3.72486100	-1.33418700	0.09913800
C	2.12926100	-2.19082800	-1.79035800
C	3.56833200	-2.07914500	-1.24520600
C	0.93216600	1.40673600	-0.64196400
C	-1.29997200	2.45628300	-0.94258000
C	-0.96189100	3.41091500	0.19468400
C	0.54876300	3.56009700	0.33559800
N	-0.53915900	1.16954500	-0.86826900
C	-0.70087200	0.47853600	-2.21708700
C	2.59335500	2.37424200	0.75257300
H	4.79651700	-1.18723400	0.28671000
H	3.36074500	-1.95636300	0.92121200
H	2.16746000	-2.70329500	-2.76088900
H	1.52649700	-2.82488000	-1.13287300
H	4.00640300	-3.07860500	-1.16621200
H	-2.36298600	2.22563000	-0.99843200
H	-1.42140300	4.37460200	-0.03577300
H	-1.37956500	3.06620800	1.14141700
H	0.78119000	4.18738600	1.19870400
H	-1.77555600	0.37675500	-2.37220300
H	-0.31637800	1.21068900	-2.92958600
H	2.72787700	3.10016600	1.55849100
H	3.06922800	2.80177300	-0.15021600
C	-0.92916100	0.27183400	0.32285700
N	0.12664000	-0.69964100	0.40954400
C	0.16149200	-1.44161000	1.70010500
N	1.14523900	2.24679900	0.52237800
H	2.99313900	0.76198100	2.10787900
H	4.37013000	1.26578300	1.15074100
H	-0.02479000	-1.05128200	-3.50334400
H	-0.50988300	-1.65495100	-1.92935500
H	2.06403700	-0.19592700	-2.56174400
H	3.39224700	0.47405900	-0.87979500
H	1.29623300	1.90699800	-1.55985000
H	0.95933400	4.06025500	-0.56257800
C	-1.20320300	-1.56131300	2.40957800
H	-1.63329900	-0.59220300	2.67249600
H	-1.93437700	-2.11873700	1.82845900
H	-1.03916700	-2.10437000	3.34195800
C	0.62092500	-2.87739300	1.42982000

H	0.68394200	-3.43875200	2.36606700
H	-0.08880400	-3.37901600	0.76746900
H	1.59908600	-2.89497100	0.95596000
C	1.11291100	-0.79422600	2.71413100
H	0.99772500	-1.25001200	3.70101600
H	2.14334600	-0.93117800	2.39966800
H	0.90982600	0.27651600	2.79311100
H	-0.93960300	0.97491800	1.16759300
C	-2.36608500	-0.21065300	0.12065700
C	-3.41777200	0.59326600	0.56530600
C	-2.67290900	-1.44145300	-0.46036300
C	-4.74393100	0.21025600	0.38398100
H	-3.19740500	1.52049000	1.08429900
C	-3.99517600	-1.82975800	-0.64464400
H	-1.86342700	-2.11152100	-0.71150300
C	-5.03624000	-1.00019600	-0.23450100
H	-5.54340100	0.84864400	0.73883600
H	-4.21320800	-2.79010200	-1.09519600
H	-6.06519600	-1.30647200	-0.37495600
H	4.16428900	-1.53891300	-1.99081100
H	-0.99514200	2.91246700	-1.88652500

cat3_im2_CP2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1126.702636	-1126.103254	-1126.075473	-1126.160119

C	-0.01897800	-0.58125100	2.42591700
C	-0.76328300	-2.37452800	-2.16189100
C	0.34511600	-1.84108300	1.63395600
C	-0.07367300	-2.83189500	-0.87323300
B	-0.53938100	-1.96959100	0.34939500
C	1.45154900	-2.95732600	-0.97484200
C	1.84266100	-2.01908100	1.35093600
C	2.10715600	-3.18492900	0.39169300
C	-2.00927300	-1.38452300	0.35672800
C	-3.57263000	0.09845900	1.39369400
C	-4.17552800	0.40722500	0.03001300
C	-3.92099500	-0.74690400	-0.93055400
N	-2.16287400	-0.23426400	1.24338900
C	-1.53315200	-0.44066900	2.54386000
C	-2.25232400	-2.14283800	-1.92884800
H	1.72217100	-3.76153000	-1.66682800
H	1.85488900	-2.03141000	-1.39708400
H	2.39116800	-2.16642400	2.28674700
H	2.23536400	-1.10155200	0.90254900
H	3.18488600	-3.31363700	0.26229100
H	-3.66130200	0.96628400	2.05253200
H	-5.24978000	0.58060500	0.12575100
H	-3.71236300	1.31288100	-0.36498200

H	-4.26393600	-0.48901800	-1.93552000
H	-1.77691400	0.42784400	3.16083900
H	-2.73774000	-1.87227900	-2.86945700
H	-2.72276400	-3.08318900	-1.58222100
N	-2.49693300	-1.05693100	-0.98476400
H	1.72502600	-4.11559300	0.82912400
H	-0.32124500	-1.43123400	-2.49991000
H	-0.62502200	-3.10531200	-2.96499000
H	0.42677100	-0.60406500	3.42539000
H	0.36941600	0.30533000	1.91417600
H	0.01143800	-2.71161600	2.23112400
H	-1.95256400	-1.32913400	3.05404600
H	-4.12286400	-0.73907000	1.86333800
H	-4.49383800	-1.63351300	-0.59692700
H	-2.63422900	-2.23644500	0.76271700
H	-0.47742200	-3.83056000	-0.62061000
C	1.21251200	1.86787100	-0.80739500
H	0.73758500	1.48849400	-1.71780700
N	0.68492000	2.74123900	-0.05730200
C	-0.62414800	3.31718400	-0.38326500
C	-1.46135100	3.19631400	0.89433800
H	-0.93049400	3.65869300	1.72814800
H	-2.42384700	3.69822800	0.76386300
H	-1.63308500	2.14139600	1.11610200
C	-1.36556800	2.65237700	-1.54547900
H	-0.83256000	2.77738800	-2.49170700
H	-1.52510800	1.58639500	-1.35837800
H	-2.34170600	3.12920900	-1.65871100
C	-0.36824900	4.79562700	-0.69677300
H	-1.31565100	5.31702200	-0.84924600
H	0.16698300	5.26508900	0.12944300
H	0.23573100	4.89458800	-1.60121900
C	2.53047300	1.27577200	-0.49525600
C	3.11729500	0.39491200	-1.40371600
C	3.18698800	1.56544400	0.70512400
C	4.33837700	-0.20827900	-1.11484800
H	2.61015400	0.17800000	-2.33801000
C	4.40455700	0.96512700	0.99264900
H	2.71515500	2.25467800	1.39343500
C	4.98087600	0.07365500	0.08636400
H	4.78309000	-0.89652800	-1.82293800
H	4.90703200	1.18487600	1.92636400
H	5.92825700	-0.39722600	0.31731700

cat3_am2_CP	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1127.908787	-1127.278807	-1127.252905	-1127.329861

C	-1.82249600	0.31521500	2.48599700
C	-1.46726900	0.72032200	-2.65396000
C	-2.53399000	0.11949500	1.14106300
C	-2.33319700	0.30691300	-1.46662200
B	-1.50867200	0.24114000	-0.09049400
C	-3.41026200	-0.76054100	-1.65159000
C	-3.61166300	-0.96077700	0.96211400
C	-4.32093900	-0.80537100	-0.40302300
C	-0.75388500	1.67410500	0.07437000
C	0.72113400	2.95651100	1.52745400
C	1.58628700	3.27969100	0.31878500
C	0.71233600	3.32052600	-0.92465000
N	-0.01165900	1.70075300	1.34857200
C	-0.98490800	1.60093300	2.45376500
C	-0.75921400	2.04485600	-2.31572000
N	0.05785800	2.03379100	-1.09437300
C	0.95597600	-0.74698000	-0.97217600
N	-0.08061900	-0.99620900	0.08131200
C	-0.19285200	-2.49602600	0.36852200
C	-0.68232100	-2.74329300	1.79529700
C	-1.14467900	-3.13553700	-0.63584700
C	1.15928200	-3.22729200	0.27490500
C	2.40072400	-0.74374500	-0.51795600
C	2.79993100	-0.12761700	0.67035400
C	3.38091400	-1.28731500	-1.35043200
C	4.14633200	-0.08253200	1.02421100
C	4.72621100	-1.23387700	-1.00321400
C	5.11406900	-0.63630800	0.19238600
H	0.76926500	0.24719800	-1.36774900
H	0.98548900	-4.26168100	0.57716500
H	1.56890100	-3.24658100	-0.73346000
H	1.90586000	-2.79910600	0.94275500
H	-0.77134300	-3.82086100	1.94501600
H	0.04416600	-2.36795300	2.52113800
H	-1.64710300	-2.29669800	1.99819400
H	-1.07903200	-4.22204600	-0.55246000
H	-3.21458300	-1.97345900	1.03769700
H	-0.88765600	-2.85866500	-1.66046800
H	3.08418900	-1.76482300	-2.27866900
H	5.46960800	-1.66577100	-1.66197000
H	6.15994300	-0.59891200	0.47027900
H	4.43876800	0.39571000	1.95121800
H	2.05885900	0.34463600	1.30703800
H	0.00740700	3.78808900	1.67547700
H	1.32723400	2.87973200	2.43492100

H	2.35816600	2.51907300	0.18864000
H	2.07358700	4.24539800	0.47035400
H	-0.03678300	4.12934000	-0.82223200
H	1.31108700	3.53244200	-1.81407800
H	-0.09997300	2.33852800	-3.13722800
H	-1.53786300	2.82601900	-2.23129100
H	-0.74020000	-0.05025200	-2.92310600
H	-2.07444000	0.89984600	-3.54963100
H	-2.92154500	1.21722500	-1.25221800
H	-4.03911800	-0.51941500	-2.51767600
H	-2.98276300	-1.74143100	-1.86081700
H	-4.88242400	0.13603300	-0.37752100
H	-5.06178400	-1.60214900	-0.51573200
H	-4.37011700	-0.88243100	1.75092100
H	-2.17053000	-2.83812000	-0.44671100
H	-3.09955900	1.05756800	1.01157800
H	-2.53561800	0.40775100	3.31414500
H	-1.16331300	-0.51189700	2.74422000
H	-1.67327800	2.46362200	2.40223000
H	-0.42354700	1.69494500	3.38747700
H	-1.56562600	2.44395100	0.15096200
H	0.27650600	-0.54963700	0.92869600
H	0.81032300	-1.47739800	-1.76741600

cat3_THF_CP	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-876.179752	-875.696491	-875.677104	-875.741369

C	0.43158500	0.74135300	2.44272700
C	0.37660100	-1.79059400	-1.94608200
C	1.10909700	-0.42710600	1.73010600
C	1.07097900	-1.77468500	-0.58485300
B	0.45959700	-0.59746300	0.29051100
C	2.60244400	-1.82781500	-0.55155300
C	2.63865900	-0.45547700	1.68200400
C	3.13685100	-1.68445900	0.89068500
C	-1.13803900	-0.67100500	0.35218400
C	-3.14331800	0.30421300	1.25594300
C	-3.77488300	0.25158100	-0.12889000
N	-1.71131800	-0.73181600	-0.99749100
C	-3.15913500	-0.88476800	-0.93418500
N	-1.69899100	0.44033800	1.13275800
C	-1.08593300	0.51929900	2.46136300
C	-1.14306600	-1.85372000	-1.75140000
H	2.96521400	-2.77799700	-0.96043000
H	3.03549600	-1.05617700	-1.19367800
H	3.06448200	-0.49714500	2.69140900
H	3.02480400	0.47137100	1.24358700
H	2.82647400	-2.57630800	1.44774000

H	4.23051500	-1.69607500	0.87693100
H	-3.53389000	1.15101800	1.82705900
H	-4.85409200	0.10549900	-0.04348200
H	-3.59754400	1.19879500	-0.64413400
H	-3.56081100	-0.89803400	-1.95122500
H	-1.57710800	1.33822200	2.99401000
H	-1.29456900	-0.40615100	3.03089300
H	-1.64085100	-1.87259800	-2.72500200
H	-1.38665700	-2.80915900	-1.24829500
H	-0.45605800	1.49763600	-2.12626600
C	-0.22491200	1.83867400	-1.11580400
C	0.47712600	3.19428100	-1.09476800
O	0.77524600	0.93314700	-0.56346100
H	-1.09759200	1.75676500	-0.48027400
C	1.98241500	2.84991200	-1.17736000
H	0.14429600	3.81877600	-1.92296200
H	0.25595500	3.71764900	-0.16526000
C	2.00699600	1.32152100	-1.20716100
H	2.46379700	3.26464400	-2.06203300
H	2.51102600	3.21906400	-0.29921200
H	2.83192800	0.88473600	-0.66180500
H	1.99612300	0.93532700	-2.23032900
H	0.67912300	-2.64748300	-2.55924300
H	0.62276900	-0.88786500	-2.51602300
H	0.65013200	1.68035300	1.92201400
H	0.77530700	0.85491000	3.47741200
H	0.80236200	-1.34226800	2.26396600
H	0.72839200	-2.67625800	-0.04965900
H	-1.38985400	-1.62823100	0.88471300
H	-3.42613500	-1.84819900	-0.45805200
H	-3.40161400	-0.61955700	1.80817500

cat4_im2_CP1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1523.807986	-1523.232628	-1523.204969	-1523.284983

C	-0.26084000	-1.72447800	-1.84284600
C	3.16850800	1.23269400	0.49803100
C	1.14164200	-1.56483100	-1.35797300
C	2.73887100	-0.13564800	0.04931200
B	1.14834800	-0.33498700	-0.27564100
C	3.44628000	-1.36559300	0.62043400
C	1.81224600	-2.83218500	-0.82229100
C	3.25816100	-2.54343800	-0.36271500
C	0.72660900	0.99038300	-1.11332100
C	-1.47306500	1.97302600	-1.75122800
C	-1.00943300	3.29295000	-1.14809400
C	0.51215800	3.37925400	-1.13180000
N	-0.76497500	0.79246200	-1.15763200

C	-1.03519800	-0.39654900	-2.05423800
C	2.50494000	2.34309300	-0.31155000
H	4.51756700	-1.17597000	0.73321400
H	3.06856300	-1.62407300	1.61049700
H	1.84317200	-3.61597400	-1.58661000
H	1.22388300	-3.22952300	0.00293300
H	3.68093500	-3.45307500	0.07165100
H	-2.54574600	1.81744100	-1.64136400
H	-1.42738800	4.09659700	-1.75784900
H	-1.38960900	3.41972400	-0.13521400
H	0.82700200	4.29103500	-0.62106700
H	-2.10537600	-0.59213500	-2.03928900
H	-0.75132200	-0.06525200	-3.05157200
H	2.74346000	3.28948000	0.17602900
H	2.98298700	2.34119600	-1.30512100
C	-1.10876800	0.53774500	0.32796400
N	-0.14914200	-0.46206100	0.70623300
C	-0.11954000	-0.82436500	2.15147600
N	1.05291700	2.22506500	-0.42568400
H	1.70361700	-1.23201400	-2.24134200
H	3.10781100	-0.09242500	-0.98973100
H	1.05829900	1.02734500	-2.16874600
H	0.89727600	3.42340100	-2.16776400
C	-1.47364900	-0.68862600	2.86999500
H	-1.84016300	0.33939200	2.88763900
H	-2.24442500	-1.32687000	2.44343300
H	-1.32116800	-0.99470900	3.90642300
C	0.27462800	-2.29785800	2.27636000
H	0.26111800	-2.60189600	3.32598700
H	-0.42687200	-2.91714800	1.71411900
H	1.27591100	-2.47342900	1.89202500
C	0.86935600	0.03775100	2.94002100
H	0.77102800	-0.15525300	4.01160200
H	1.89278400	-0.17149900	2.65115600
H	0.68606100	1.09896800	2.75985300
H	-0.92518400	1.51720200	0.78993000
C	-2.61032500	0.28002400	0.43306100
C	-3.43206200	1.34784000	0.80162500
C	-3.20245500	-0.95717900	0.17152500
C	-4.81374000	1.20016000	0.87952700
H	-2.98384100	2.30214800	1.05746300
C	-4.58347500	-1.10720900	0.24540400
H	-2.57370700	-1.80234300	-0.06250500
C	-5.39446400	-0.03037100	0.59360600
H	-5.43032600	2.04005700	1.17427100
H	-5.02576900	-2.07449800	0.04182600
H	-6.46836000	-0.15428000	0.65587800
H	3.85609000	-2.32068800	-1.25442100

H	-1.21995500	1.95937100	-2.81294700
F	2.99526600	1.49379200	1.82968900
F	4.52963000	1.39621300	0.29247500
F	-0.97851400	-2.58504700	-1.05588200
F	-0.32971600	-2.30308900	-3.10253900

cat4_im2_CP2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1523.828321	-1523.259677	-1523.22917	-1523.319094

C	-0.60243800	-1.30614400	-1.42632400
C	3.64570000	0.53224600	0.50554600
C	0.87792400	-1.67540200	-1.35733100
C	3.18869900	-0.66340700	-0.33577600
B	1.74843200	-0.45621100	-0.92116600
C	3.33120900	-2.00744200	0.33816000
C	1.17693200	-2.94810300	-0.55532700
C	2.68599800	-3.16230900	-0.39912800
C	1.28925600	1.00484600	-1.28709400
C	-0.53737900	2.45019600	-1.91267700
C	0.02685900	3.51990300	-0.98933100
C	1.52897200	3.33940100	-0.82592300
N	-0.16987700	1.13571000	-1.37509700
C	-0.79958900	0.05940500	-2.04180300
C	3.27407600	1.83428900	-0.19671300
H	0.72640300	-3.82329900	-1.02969900
H	0.73335500	-2.86017800	0.43979900
H	2.90233000	-4.07056300	0.16552100
H	-1.62146600	2.51765100	-1.96546100
H	-0.18609700	4.51039100	-1.39713300
H	-0.44641200	3.42895300	-0.01136900
H	1.92086800	4.05735800	-0.10172500
H	3.62931100	2.67911600	0.39713500
H	3.78918500	1.89080800	-1.17563600
N	1.83104700	1.99286100	-0.35476300
H	3.16835500	-3.25143800	-1.37662000
H	3.14483600	0.50541600	1.47331000
H	4.72334500	0.49405000	0.67841800
H	-1.17086400	-2.01406800	-2.03359000
H	-1.05360800	-1.27984900	-0.43280900
H	1.22717400	-1.83459300	-2.39357200
H	-0.13158400	2.57369000	-2.92811500
H	2.02927200	3.53130800	-1.79511400
H	1.72154700	1.19859200	-2.30651300
H	3.81913400	-0.71551600	-1.23915500
C	-2.73438200	0.40356500	1.22178300
H	-3.34938500	1.26967000	0.95927700
N	-3.08316700	-0.79212900	0.98587200
C	-4.38371000	-1.08571400	0.37178400

C	-4.12177200	-2.08551600	-0.75873300
H	-3.53105900	-2.92214000	-0.38178000
H	-5.06728400	-2.46636000	-1.15087700
H	-3.57514300	-1.60278500	-1.56843000
C	-5.13727700	0.12252000	-0.18921700
H	-5.43611500	0.82106400	0.59570900
H	-4.52697600	0.64998000	-0.92539300
H	-6.04595600	-0.22400000	-0.68432000
C	-5.21856100	-1.76266200	1.46536400
H	-6.17775400	-2.09075900	1.05909000
H	-4.68510300	-2.62803600	1.86018600
H	-5.40369400	-1.06716700	2.28631100
C	-1.45865500	0.72974700	1.88957100
C	-1.18673000	2.05763900	2.21580500
C	-0.53170500	-0.26274700	2.22092700
C	0.00082900	2.40022300	2.85409500
H	-1.91412900	2.82446200	1.96987300
C	0.65630800	0.07790600	2.85386100
H	-0.77385000	-1.29357600	1.99331700
C	0.92418600	1.41065500	3.16953100
H	0.20356700	3.43472800	3.10278500
H	1.37522500	-0.69191600	3.09899100
H	1.85183400	1.67203900	3.66412500
F	2.76226900	-1.93939300	1.59546600
F	4.65817100	-2.28935800	0.55195900
F	-2.14400300	0.32150800	-2.10836600
F	-0.39042900	-0.00338600	-3.37451500

cat4_am2_CP	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1525.024242	-1524.425181	-1524.396215	-1524.480069

C	-1.05159800	-1.16405800	2.38425700
C	-1.87496400	1.75797400	-1.67364600
C	-1.98608200	-0.83914300	1.25351700
C	-2.41070100	0.66933300	-0.79942500
B	-1.23219200	0.04727900	0.12598400
C	-3.51429400	-0.25260600	-1.32076300
C	-2.99999800	-1.85524000	0.71013900
C	-4.05036800	-1.11847300	-0.15502700
C	-0.63726600	1.33801400	0.93887800
C	1.04162800	1.96117300	2.60858100
C	1.60708400	2.96231200	1.61459100
C	0.47356300	3.49893300	0.75227900
N	0.35715400	0.86877700	1.91613100
C	-0.33686800	0.06907500	2.92751400
C	-1.18061800	2.85561700	-0.86454200
N	-0.14187400	2.38799800	0.04494200

C	1.19759600	0.11316500	-1.16278000
N	0.20190300	-0.83137500	-0.55349700
C	0.15492000	-2.15630700	-1.35835800
C	0.01818700	-3.35440500	-0.41612200
C	-0.99709400	-2.10333900	-2.35052200
C	1.44736500	-2.42930600	-2.15185200
C	2.64333300	-0.13097500	-0.79504700
C	3.04262200	-0.51995500	0.48661400
C	3.62904400	0.12287500	-1.75199600
C	4.39349300	-0.67663400	0.78782700
C	4.97786600	-0.02041400	-1.44788700
C	5.36602600	-0.42955000	-0.17537800
H	0.93708300	1.11568600	-0.83550700
H	1.32544300	-3.41462400	-2.60453400
H	1.61940100	-1.72188200	-2.96164400
H	2.32840800	-2.46071200	-1.51466900
H	-0.12089600	-4.24796800	-1.02763500
H	0.92914000	-3.48249500	0.17172400
H	-0.81088800	-3.27694100	0.27360500
H	-0.87047200	-2.89261300	-3.09374000
H	-2.53066800	-2.63512100	0.11464500
H	-1.02804700	-1.14032200	-2.86161600
H	3.33147500	0.42600500	-2.75018100
H	5.72435800	0.17728600	-2.20737000
H	6.41494200	-0.55247100	0.06287500
H	4.68502200	-0.98709800	1.78370400
H	2.30300100	-0.67599000	1.26352800
H	0.33766900	2.48850100	3.27889600
H	1.83453800	1.53379100	3.22791000
H	2.34936200	2.47354600	0.97905000
H	2.09224100	3.77877200	2.15278100
H	-0.26417300	4.01937100	1.39211700
H	0.84481200	4.21773100	0.01794400
H	-0.73666600	3.55859000	-1.57245300
H	-1.98475800	3.38167700	-0.32287800
H	-2.93049600	1.24747300	-0.02025000
H	-4.34187100	0.35326300	-1.69977400
H	-3.18725200	-0.86587500	-2.15516000
H	-4.61669300	-0.45699600	0.51126700
H	-4.76607400	-1.84635800	-0.54492400
H	-3.51709200	-2.35841900	1.53195600
H	-1.94507700	-2.26713300	-1.84845900
H	-2.61980000	-0.07433800	1.72646600
H	-1.09339200	0.67125200	3.45758800
H	0.38999500	-0.28288200	3.66255600
H	-1.49066500	1.77895500	1.51744600
H	0.59644800	-1.08975300	0.34912300
H	1.06164500	0.09977000	-2.23963400

F	-1.00590800	1.26427900	-2.62837600
F	-2.86954000	2.38428200	-2.39096200
F	-0.06093500	-2.07117800	2.02873600
F	-1.69990400	-1.75452300	3.44139700

cat4_THF_CP	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1273.302477	-1272.849899	-1272.827658	-1272.898063

C	1.87136800	-1.46888800	-0.87021800
C	-1.63387500	2.06273500	-0.25334700
C	1.50654600	-0.07321500	-1.27223800
C	-0.34011300	1.78481700	-0.95547700
B	0.17080900	0.33922300	-0.49199800
C	0.74815700	2.86251300	-0.94016700
C	2.59647300	1.00008100	-1.24301700
C	2.01063700	2.36244100	-1.68144100
C	-0.97403700	-0.75970000	-0.72650300
C	-1.52437800	-3.10567800	-0.56617800
C	-2.79115100	-2.73849400	0.19606300
N	-2.19034900	-0.37901400	-0.00022600
C	-3.25816400	-1.34867200	-0.21538800
N	-0.50193900	-2.09317200	-0.33482600
C	0.71829900	-2.45172300	-1.04931100
C	-2.65145900	0.93931500	-0.42369400
H	0.39344000	3.76964100	-1.43675000
H	0.98548500	3.15838600	0.08267100
H	3.41033100	0.73834700	-1.92466000
H	3.05211000	1.05913400	-0.25220000
H	1.74964500	2.27286100	-2.74239000
H	2.78889100	3.12747100	-1.62211200
H	-1.14280900	-4.07606400	-0.23890200
H	-3.57519800	-3.46949400	-0.01177600
H	-2.58810600	-2.75100300	1.26933800
H	-4.13276600	-1.04685600	0.36615400
H	1.06064100	-3.42599300	-0.69483300
H	0.54502200	-2.52996000	-2.13650000
H	-3.53362300	1.20870700	0.16061300
H	-2.93904300	0.94543500	-1.48943200
H	-1.00472800	0.14953800	2.55556600
C	-0.17365600	-0.44747600	2.18225600
C	0.93173400	-0.66766500	3.21674900
O	0.47566700	0.34851300	1.14246200
H	-0.52680700	-1.35118300	1.70693400
C	1.97325700	0.43679900	2.92938000
H	0.52737700	-0.60236200	4.22603900
H	1.37940700	-1.65051900	3.08463900
C	1.30262600	1.29415300	1.86634100

H	2.22408100	1.02712800	3.80950900
H	2.88427500	-0.00100200	2.52638300
H	1.98860900	1.75056600	1.16784400
H	0.63631400	2.04866200	2.28698900
H	1.17854400	-0.16555300	-2.31780400
H	-0.62463500	1.63300600	-2.00639200
H	-1.20638000	-0.77852200	-1.82533400
H	-3.55453700	-1.36761200	-1.28146700
H	-1.75756900	-3.18212300	-1.64494500
F	-1.42660500	2.28506100	1.09447700
F	-2.23723400	3.21295400	-0.71383100
F	2.30521700	-1.51057700	0.43951700
F	2.92474200	-1.96050700	-1.61065100

cat3_im1_CP1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-856.300125	-855.805397	-855.786285	-855.847675

C	0.70679900	-2.15308600	-1.33475800
C	1.02069600	2.51294700	0.70046700
C	1.61022600	-0.92282500	-1.24069400
C	1.80095000	1.43168400	-0.04354100
B	0.89249700	0.11465900	-0.22057400
C	3.21838400	1.09730200	0.42207800
C	3.00230000	-1.23105000	-0.68190000
C	3.84266400	0.04862200	-0.51862000
C	-0.54319900	0.54079700	-0.82975100
C	-2.78958800	-0.55560200	-0.85105000
C	-3.39008800	0.81377100	-0.51127400
C	-2.43474700	1.96990000	-0.80863300
N	-1.33510000	-0.72361600	-0.52131500
C	-0.78217900	-1.79182300	-1.46734500
C	-0.26346800	2.82671400	-0.07528600
H	3.85661500	1.99016500	0.43535300
H	3.21584600	0.71217900	1.44643100
H	3.55498300	-1.94847700	-1.30238100
H	2.87462900	-1.70194000	0.30191100
H	4.84505000	-0.21303400	-0.16698500
H	-3.34480100	-1.36542900	-0.37517700
H	-4.30313600	0.91357700	-1.10324400
H	-3.67494000	0.86165600	0.53632900
H	-2.84546500	2.89121500	-0.38976900
H	-1.42658300	-2.66444500	-1.35480700
H	-0.95444300	-1.37554900	-2.46068900
H	-0.82891800	3.61796200	0.42481500
H	0.01201800	3.20660800	-1.07528300
C	-1.00511500	-1.06969400	0.96716100
N	0.38318800	-0.70506000	1.04372300

N	-1.15988100	1.67222500	-0.18712900
H	1.72032800	-0.46937600	-2.23725900
H	1.92186000	1.81014700	-1.07447700
H	-0.58567800	0.63880100	-1.93061800
H	-2.32926400	2.11638800	-1.89939000
H	3.96806400	0.50683200	-1.50727700
H	-2.85250900	-0.69925600	-1.93072000
C	0.93897500	-0.64450800	2.37333600
H	0.67353500	0.25655600	2.94887600
H	0.63962700	-1.51125100	2.97678100
H	2.02523800	-0.68026000	2.31067600
C	-1.28838700	-2.56442200	1.21989400
H	-0.65511600	-3.22761100	0.64059500
H	-1.08831700	-2.75752600	2.27420500
H	-2.33824100	-2.81647100	1.04668600
C	-1.90574500	-0.30971000	1.95885400
H	-2.95248200	-0.60996200	1.87837700
H	-1.57429200	-0.59532700	2.95783100
H	-1.79847100	0.76311000	1.84127300
H	0.92631300	-2.79277900	-2.19908400
H	0.86802300	-2.75536200	-0.44221800
H	1.58951300	3.44571100	0.80371700
H	0.75021100	2.18090100	1.70780400

cat3_im1_CP2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-856.295323	-855.802091	-855.782003	-855.846304

C	0.65757000	0.76024200	2.39056500
C	0.46790600	-1.58234000	-2.12362600
C	1.34864500	-0.29398200	1.52866700
C	1.26707800	-1.48181500	-0.82715400
B	0.63870200	-0.30406900	0.07380700
C	2.79664700	-1.55945400	-0.85899200
C	2.87962100	-0.41136300	1.54510500
C	3.35778900	-1.53492800	0.58748000
C	-0.90891200	-0.69187900	0.33809900
C	-2.93038200	-0.10900300	1.51822700
C	-3.72766300	-0.34175300	0.24244700
C	-3.01479400	-1.37088900	-0.62522400
N	-1.56164500	0.29408700	1.21397200
C	-0.83729800	0.41821000	2.48795300
C	-0.99077200	-1.90801000	-1.77085600
H	3.22042000	-0.67847800	2.55280800
H	3.37893600	0.53371300	1.32390400
H	4.45119200	-1.54825500	0.55929900
H	-3.40045800	0.66372600	2.13386200
H	-4.72898000	-0.69807800	0.49500600

H	-3.83188700	0.59532600	-0.30846800
H	-3.54470800	-1.51528600	-1.57104000
H	-1.59124400	-1.98820200	-2.68176000
H	-1.00322500	-2.90371000	-1.28859900
N	-1.65633000	-0.92920400	-0.90540500
H	3.05349700	-2.48292900	1.04550000
H	0.50846700	-0.64133800	-2.68467400
H	0.83405100	-2.37363600	-2.78913800
H	1.05227800	0.79949400	3.41320200
H	0.77757200	1.76372500	1.96480900
H	-2.93060100	-1.04672900	2.10784200
H	-3.00413100	-2.34385300	-0.09694200
H	-0.88531500	-1.66765500	0.89266100
C	0.03208600	2.18513400	-0.99990200
N	0.84028100	1.24865300	-0.62394900
C	-1.43807100	2.04206000	-1.18708500
H	-1.93709000	2.35574900	-0.26774400
H	-1.74374800	2.70174200	-2.00184800
H	-1.71278600	1.00772700	-1.38036500
C	2.26021900	1.63824400	-0.65021400
H	2.49826900	2.28708000	0.19518900
H	2.86628500	0.75435100	-0.57982400
H	2.50408500	2.15233000	-1.57898900
H	1.01469300	-1.26275900	1.93231100
H	0.98047400	-2.37226400	-0.24329000
C	0.54043600	3.57350800	-1.32325800
H	1.30882000	3.91657100	-0.63315000
H	0.96087700	3.59519500	-2.33332000
H	-0.29372000	4.27098500	-1.29723800
H	3.24493300	-0.78292900	-1.48617900
H	3.11735200	-2.50354400	-1.31616500
H	-0.91699500	-0.53258500	3.04907000
H	-1.35760300	1.17822300	3.07851800

cat3_am1_CP	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-857.526338	-857.007848	-856.987502	-857.051992

C	-0.06614200	2.70190300	-0.87728500
C	0.49981200	-1.54145000	2.05577200
C	0.78119100	1.96619800	0.16273100
C	1.05809000	-0.16078600	1.67960800
B	0.35347800	0.43236400	0.35903900
C	2.57851600	0.06008400	1.69194200
C	2.30034800	2.12691700	0.12272300
C	2.92468500	1.53713100	1.40462200
C	-1.25111900	0.35560300	0.55351300

C	-3.35807300	0.82733600	-0.54013600
C	-3.71116500	-0.65071700	-0.45988700
C	-3.06046000	-1.25776200	0.77339100
N	-1.91097900	0.97521500	-0.60218400
C	-1.55776200	2.40237300	-0.65026700
C	-1.03517700	-1.53275500	2.00507500
N	-1.61352300	-1.06233200	0.73352300
C	1.67415300	-1.66350100	-1.02238300
N	0.57392800	-0.63692800	-1.00254800
H	1.96758800	-1.80922700	0.00815100
H	2.71521200	1.62743800	-0.76105800
H	-3.76905700	1.34920100	0.34513300
H	-3.80042100	1.28480400	-1.42919400
H	-3.33988500	-1.15655200	-1.35473400
H	-4.79431600	-0.78113700	-0.41193900
H	-3.48495200	-0.77731000	1.67368300
H	-3.27000500	-2.32884200	0.84020100
H	-1.41257800	-2.54383300	2.18025100
H	-1.41290600	-0.90020900	2.82779700
H	0.66927200	0.51294400	2.46086900
H	3.01039300	-0.21719000	2.66146900
H	3.08890100	-0.56336700	0.95140000
H	2.57038600	2.13944200	2.24941000
H	4.01199300	1.65308700	1.37510200
H	2.59706400	3.18010700	0.04223200
H	0.46835300	2.40206700	1.12722400
H	-1.86647000	2.88685300	0.29502600
H	-2.15117600	2.85741700	-1.44827000
H	-1.55890600	0.91139100	1.47413600
H	-0.28205800	-1.17209900	-0.79594100
C	1.13419300	-2.99225200	-1.54960700
H	1.91056900	-3.75632000	-1.48756900
H	0.28015700	-3.32331900	-0.95390800
H	0.82209100	-2.92006900	-2.59342600
C	0.38726500	-0.05712000	-2.35301500
H	0.39585700	-0.84515800	-3.10858900
H	-0.57114100	0.44912500	-2.36268000
H	1.19018000	0.64530400	-2.56295500
C	2.91188500	-1.21841800	-1.79258300
H	3.27114000	-0.24798400	-1.45216100
H	3.70386400	-1.94875400	-1.61831600
H	2.73511200	-1.17261300	-2.86786400
H	0.21399900	2.44141500	-1.89857200
H	0.06434300	3.78797800	-0.79624400
H	0.79722500	-1.83462500	3.06973400
H	0.85536500	-2.34018100	1.39958200

cat4_im1_CP1	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1253.414127	-1252.950565	-1252.928429	-1252.996211

C	1.71796800	1.77193400	-0.73690700
C	-2.62605700	-0.70516400	-0.09972800
C	0.22709100	1.88647100	-0.88420400
C	-2.01972100	0.62461100	-0.40955600
B	-0.41884400	0.56016200	-0.19352700
C	-2.63954200	1.87990200	0.20219200
C	-0.39370800	3.12386400	-0.22481900
C	-1.92738200	3.11900600	-0.37664700
C	0.16533700	-0.75536500	-0.93574400
C	2.26526800	-2.08412300	-0.64097500
C	1.40182900	-3.34755800	-0.72216700
C	0.03893900	-3.09134300	-1.36483400
N	1.52848300	-0.82948700	-0.26186500
C	2.30538700	0.33909600	-0.83675200
C	-2.00217400	-1.82882700	-0.92243500
H	-3.70823800	1.94109700	-0.02313000
H	-2.54884800	1.86274300	1.29009100
H	0.00434700	4.05449300	-0.64194100
H	-0.12718400	3.11666400	0.83494700
H	-2.33524300	4.02244200	0.08412400
H	3.09808500	-2.21268900	0.05127100
H	1.96583100	-4.07599800	-1.30926300
H	1.24494800	-3.77349800	0.26467700
H	-0.58799500	-3.97736900	-1.24689200
H	3.30813900	0.33420200	-0.41523900
H	2.37766000	0.13925200	-1.90373300
H	-2.49117400	-2.76109700	-0.63356700
H	-2.24046000	-1.63058800	-1.97909700
C	1.25594300	-0.62652400	1.26885800
N	0.23107500	0.37415700	1.22067500
N	-0.57147300	-1.96502600	-0.68560600
H	0.03003400	1.90581400	-1.96400400
H	-2.14250500	0.72166800	-1.49957900
H	0.38859900	-0.64294300	-2.01337600
H	0.14779400	-2.89740500	-2.44732000
H	-2.16818100	3.17948400	-1.44499900
H	2.67908500	-1.88491400	-1.63040600
F	-2.50992400	-1.02571000	1.23266500
F	-3.98080200	-0.73993800	-0.36579200
F	2.17335100	2.37321800	0.40607900
F	2.40055900	2.42781000	-1.75154000
C	-0.34429600	0.74064500	2.49559800
H	-1.10677900	0.04011000	2.85726800
H	0.42949700	0.83330500	3.26585200
H	-0.81055400	1.72139500	2.41665300

C	2.55984900	-0.17661200	1.95445400
H	2.84396500	0.83085100	1.67364300
H	2.39172600	-0.19114000	3.03104200
H	3.38024300	-0.87341600	1.76186800
C	0.82370200	-1.92384900	1.97299100
H	1.62680800	-2.66305900	2.01391900
H	0.60538800	-1.63858700	3.00294900
H	-0.07661800	-2.33453100	1.53078000

cat4_im1_CP2	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1253.418912	-1252.956662	-1252.933566	-1253.004481

C	-0.54909800	-2.12530800	-1.03662300
C	1.47370900	2.21963800	0.66036400
C	0.64525200	-1.19176000	-1.20974200
C	1.68661000	1.04935500	-0.29270100
B	0.51293900	-0.03622600	-0.08779600
C	3.06444600	0.50851800	-0.53694300
C	2.05122900	-1.77413000	-1.41964000
C	3.09627400	-0.63763200	-1.55293700
C	-0.84522500	0.75863300	-0.45382900
C	-3.25434900	0.55289100	-0.80826300
C	-3.45449300	1.78323200	0.06441400
C	-2.23367800	2.68813800	-0.03221100
N	-2.01591300	-0.14005200	-0.41493300
C	-1.83774900	-1.32451900	-1.19026500
C	0.12313300	2.85883600	0.30527500
H	2.08574600	-2.34548000	-2.35337800
H	2.34463300	-2.47806300	-0.64189900
H	4.11263600	-1.03703400	-1.55340600
H	-4.08762900	-0.14098200	-0.70906200
H	-4.34185600	2.32265900	-0.27359200
H	-3.61557400	1.48862300	1.10321200
H	-2.34782700	3.56389000	0.61225200
H	-0.08579700	3.69472900	0.97794800
H	0.21108300	3.27897200	-0.71383000
N	-1.03703900	1.96029100	0.37105400
H	2.94576900	-0.15023900	-2.51951700
H	1.46715500	1.88003400	1.70021100
H	2.24883300	2.98455200	0.56175800
H	-0.61416100	-2.91633700	-1.78891000
H	-0.56861800	-2.60020400	-0.05203000
H	-3.19172200	0.86696700	-1.85866700
H	-2.13274200	3.04940200	-1.07322600
H	-0.72737800	1.10476900	-1.50790100
C	-0.40242600	-0.88151300	2.37654100
N	0.48369700	-0.79098900	1.43746700

F	3.69982500	0.13563000	0.63784900
F	3.88082800	1.50467500	-1.03798000
F	-2.89898000	-2.15542000	-0.93182700
F	-1.95605400	-1.03185400	-2.54691900
C	-1.61649800	-0.03239500	2.52302800
H	-2.46411100	-0.56305900	2.08286000
H	-1.80600000	0.10404400	3.58963800
H	-1.50280100	0.91850800	2.01034100
C	1.64673200	-1.67814600	1.62911300
H	1.39313700	-2.70439200	1.35642700
H	2.46098000	-1.33431500	1.01968800
H	1.98051100	-1.65232800	2.66434300
H	0.44549300	-0.64436000	-2.14100200
H	1.44178700	1.42968400	-1.29574300
C	-0.26755700	-1.90306800	3.48411000
H	0.11718700	-2.86033200	3.13922100
H	0.40594300	-1.52692000	4.26020400
H	-1.24302200	-2.05830900	3.93968200

cat4_am1_CP	Energy **(E)**	Energy**(E)**+ZPE	Enthalpy **(H)**	Gibbs free energy **(G)**
IEFPCM (THF)	-1254.646521	-1254.158932	-1254.135592	-1254.206336

C	-2.46547400	-0.89418800	-0.52465200
C	2.55963000	-0.24239200	-0.60254800
C	-1.13665600	-1.55241700	-0.72548700
C	1.43107900	-1.21299700	-0.75336000
B	0.04892600	-0.56803900	-0.21648800
C	1.66378100	-2.68387700	-0.39176200
C	-0.95340400	-2.99512600	-0.25279000
C	0.41354400	-3.52450800	-0.74510400
C	-0.14825800	0.84728600	-0.95763800
C	-1.65369300	2.72957500	-1.22169700
C	-0.52520000	3.66032900	-0.80020700
C	0.81153600	3.05848000	-1.20941200
N	-1.46324200	1.41388900	-0.62153800
C	-2.52262200	0.52241000	-1.08448000
C	2.21827000	1.15598500	-1.11451500
N	0.97047400	1.73413200	-0.61790300
C	-0.16379100	0.99840500	2.11843900
N	-0.11740100	-0.38449000	1.48016500
H	-0.46956100	1.66022100	1.32100100
H	-1.03291400	-3.06121900	0.83663100
H	-1.66241400	2.65273200	-2.32560300
H	-2.62350800	3.12412200	-0.90816500
H	-0.54958000	3.80442000	0.28265900
H	-0.65267000	4.63488900	-1.27560000
H	0.85091900	2.99465600	-2.31370500

H	1.64080300	3.69179700	-0.88423000
H	3.04706300	1.81225000	-0.84000100
H	2.20375800	1.07479300	-2.21537600
H	1.25695600	-1.20416000	-1.83996200
H	2.51288100	-3.08014900	-0.95567200
H	1.92249900	-2.80211500	0.65973900
H	0.35549900	-3.58328200	-1.83811600
H	0.55674400	-4.54815100	-0.39040800
H	-1.74111300	-3.64159800	-0.64979300
H	-1.02070000	-1.56005100	-1.81805500
H	-2.50376800	0.41313600	-2.18279300
H	-3.49022600	0.94586100	-0.80711400
H	-0.12764500	0.67609500	-2.06804900
H	-1.08082000	-0.69703400	1.57025100
F	2.98887100	-0.15819200	0.71007000
F	3.67845100	-0.64319500	-1.30161700
F	-2.80021300	-0.85758300	0.83163600
F	-3.49365900	-1.59418800	-1.10721600
C	-1.25191500	1.01170900	3.18958600
H	-1.32274100	2.01429400	3.61395300
H	-2.22069300	0.75927700	2.75482700
H	-1.04094600	0.32362100	4.01217000
C	0.67264800	-1.31405000	2.32712600
H	0.41248100	-1.16890100	3.37538900
H	0.44409100	-2.33729400	2.05029800
H	1.72908400	-1.12518900	2.17965100
C	1.17797500	1.46539200	2.65909300
H	1.94949900	1.39675800	1.89913700
H	1.07033900	2.51291500	2.94732800
H	1.48747100	0.91112500	3.54755300