

Supporting Information

- S1 Table S1.** M05-2X/6-31(d) and B3LYP/6-31(d) total and relative energies of the stationary points involved in the IMDA reactions of **1** and **1w**.
- S2 Table S2.** M05-2X/6-31(d) and B3LYP/6-31(d) total and relative free energies for the stationary points involved in the IMDA reaction of **1**.
- S2 Table S3.** M05-2X/6-32G(d) total and relative free energies of the stationary points involved in the IMDA reactions of **1** and **1w**.
- S4 Table S4.** M05-2X/6-311+G(d,p)/M05-2X/6-32G(d) total and relative activation free energies in water of the stationary points involved in the IMDA reaction **1w**.
- S4** M05-2X/6-31G(d) computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved uncatalyzed and water catalyzed reactions of **1**.

Table S1. Total (E, in au) and relative ^a (ΔE , in kcal/mol) energies of the stationary points involved in the IMDA reaction of **1** and **1w**.

	M05-2X/6-31(d)		B3LYP/6-31(d)	
	E	ΔE	E	ΔE
1	-1042.543999		-1042.686309	
TS1n	-1042.517296	16.76	-1042.642032	27.8
TS1x	-1042.506665	23.43	-1042.635465	31.9
TS2n	-1042.513860	18.91	-1042.641058	28.4
TS2x	-1042.509004	21.96	-1042.639008	29.7
3	-1042.597937	-33.85	-1042.716055	-18.7
4	-1042.607228	-39.68	-1042.716131	-18.7
5	-1042.599086	-34.57	-1042.713202	-16.9
2	-1042.608707	-40.60	-1042.713229	-16.9
1w	-1271.766477		-1271.947033	
TS1nw	-1271.752046	9.06	-1271.915943	19.5
TS1xw	-1271.739294	17.06	-1271.905249	26.2
TS2nw	-1271.746151	12.75	-1271.913825	20.8
TS2xw	-1271.743739	14.27	-1271.907296	24.9
3w	-1271.831450	-40.77	-1271.980356	-20.9
4w	-1271.839078	-45.56	-1271.986505	-24.8
5w	-1271.830886	-40.42	-1271.976899	-18.7
2w	-1271.839265	-45.68	-1271.988222	-25.8

^a Relative to **1** or **1w**.

Table S2. Total (G, in au) and relative (ΔG , in kcal/mol, relative to **1**) free energies of the stationary points involved in the IMDA reaction of **1**.

	M05-2X/6-31G(d)		B3LYP/6-31(d)		M05-2X/6-31G(d)/B3LYP /6-31(d)	
	G	ΔG	G	ΔG	G	ΔG
1	-1042.152587		-1042.305227		-1042.146712	
TS1n	-1042.116588	22.6	-1042.252174	33.3	-1042.110583	22.7
TS1x	-1042.106244	29.1	-1042.245400	37.5	-1042.102081	28.0
TS2n	-1042.115550	23.2	-1042.250393	34.4	-1042.107928	24.3
TS2x	-1042.108741	27.5	-1042.249661	34.9	-1042.105609	25.8
3	-1042.192378	-25.0	-1042.312786	-4.7	-1042.189695	-27.0
4	-1042.200722	-30.2	-1042.324497	-12.1	-1042.200091	-33.5
5	-1042.193518	-25.7	-1042.315931	-6.7	-1042.190981	-27.8
2	-1042.203653	-32.0	-1042.327647	-14.1	-1042.200231	-33.6

Table S3. M05-2X/6-32G(d) total (G, in au) and relative ^a (ΔG , in kcal/mol) free energies of the stationary points involved in the IMDA reactions of **1** and **1w**.

	gas phase		in water	
	G	ΔG	G	ΔG
1	-1042.152587		-1042.160721	
TS1n	-1042.116588	22.6	-1042.128293	20.3
TS1x	-1042.106244	29.1	-1042.114524	29.0
TS2n	-1042.115550	23.2	-1042.124032	23.0
TS2x	-1042.108741	27.5	-1042.119031	26.2
3	-1042.192378	-25.0	-1042.203835	-27.1
4	-1042.200722	-30.2	-1042.211380	-31.8
5	-1042.193518	-25.7	-1042.203543	-26.9
2	-1042.203653	-32.0	-1042.211384	-31.8
1w	-1271.312651		-1271.336051	0.0
TS1nw	-1271.290386	14.0	-1271.307670	17.8
TS1xw	-1271.276130	22.9	-1271.294950	25.8
TS2nw	-1271.280983	19.9	-1271.303063	20.7
TS2xw	-1271.279108	21.0	-1271.300125	22.5
3w	-1271.362218	-31.1	-1271.385108	-30.8
4w	-1271.367543	-34.4	-1271.389476	-33.5
5w	-1271.359593	-29.5	-1271.380442	-27.9
2w	-1271.369113	-35.4	-1271.388153	-32.7

^a Relative to **1** or **1w**.

Table S4. M05-2X/6-311+G(d,p)//M05-2X/6-32G(d) total (G, in au) and relative (ΔG , in kcal/mol, relative to **1**) activation free energies in water of the stationary points involved in the IMDA reaction **1w**.

	G	ΔG
1w	-1271.753130	
TS1nw	-1271.724829	17.8
TS1xw	-1271.713641	24.8
TS2nw	-1271.721860	19.6
TS2xw	-1271.715968	23.3
3w	-1271.796581	-27.3
4w	-1271.802322	-30.9
5w	-1271.790835	-23.7
2w	-1271.804916	-32.5

M05-2X/6-31G(d) computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved uncatalyzed and water catalyzed reactions of **1**.

1

E(RM052X) = -1042.543999 a.u.

C	0.00528700	-0.01499400	-0.01099700
H	0.00190400	-0.01257800	1.08329800
C	1.50362800	-0.01524900	-0.41484900
H	1.88457300	1.00286300	-0.27886600
H	2.03931800	-0.65616400	0.28674200
C	-0.72564700	1.21143900	-0.50950900
H	-0.24779700	1.76593600	-1.30978900
C	-1.89568100	1.66028200	-0.04602400
C	1.83744700	-0.48999800	-1.83903500
H	1.44819900	-1.50454400	-1.97469800
C	3.36321400	-0.53400400	-2.00726500
H	3.81813100	-1.17906100	-1.25244200
H	3.63150200	-0.90883500	-2.99603100
H	3.78824100	0.46734000	-1.89688900
C	1.24343300	0.38760500	-2.90444700
H	1.52766200	1.43802600	-2.86560500
C	0.42239000	-0.03039800	-3.87420200
H	0.10168900	-1.07024500	-3.86654600
C	-0.14696400	0.81233000	-4.93506800
H	-1.17802800	0.59324400	-5.19783600
C	0.47454900	1.78193800	-5.61823900
H	-0.10852700	2.31580600	-6.36247800
C	-0.64814600	-1.31278500	-0.42620200
C	-1.56870200	-1.43066500	-1.38929400
H	-1.93624800	-0.57399100	-1.93960000
C	-2.09012000	-2.74028200	-1.82631500
C	-0.21009000	-2.54684800	0.30825000
C	-0.75238500	-3.86948600	-0.07626600
C	-1.66751600	-3.96043100	-1.06353200
O	-2.81612600	-2.82686300	-2.80051100
O	0.57479600	-2.45440400	1.23855900
C	-2.68967800	0.97174600	1.03168500

H	-2.12908300	0.18476300	1.53417200
H	-3.02024100	1.69460400	1.78246400
H	-3.59067100	0.52049200	0.60396700
C	-2.53296900	2.90316100	-0.60817800
H	-2.66119100	3.65811600	0.17313700
H	-1.93352700	3.33296900	-1.41074000
H	-3.52958400	2.68176000	-1.00179000
C	1.91356200	2.19151300	-5.49867200
H	2.33052400	2.39740200	-6.48662000
H	2.02099200	3.10777900	-4.90970400
H	2.50881600	1.41380700	-5.01979800
C	-0.24166100	-5.05057300	0.69021800
H	-0.31738700	-4.86012800	1.76118300
H	-0.79961300	-5.94576900	0.42947500
H	0.81601200	-5.21393800	0.47224700
O	-2.11524300	-5.16911000	-1.45101500
C	-3.47218300	-5.33364900	-1.88970600
H	-3.72668900	-6.36209400	-1.64386300
H	-4.13757000	-4.65331000	-1.35947100
H	-3.55289200	-5.16283700	-2.95833600

1w

E(RM052X) = -1271.766477 a.u.

C	0.02307200	0.01056700	-0.00244400
H	0.01914500	0.02388900	1.09156000
C	1.52488400	-0.03224700	-0.39491300
H	1.94888000	0.95237900	-0.17036500
H	2.02061000	-0.74816700	0.26450500
C	-0.69126300	1.24476000	-0.50784200
H	-0.18525200	1.82175700	-1.27183800
C	-1.88519100	1.66928100	-0.08436500
C	1.86477700	-0.40226700	-1.85011700
H	1.38054800	-1.35185900	-2.09999100
C	3.38379700	-0.58367000	-1.97729300
H	3.74524800	-1.35299300	-1.29140500
H	3.65340300	-0.86885300	-2.99509400
H	3.89997200	0.35035200	-1.73952600
C	1.39578200	0.63926700	-2.82653000
H	1.82283300	1.63292600	-2.69604100
C	0.49323600	0.44207400	-3.79233300
H	0.01593400	-0.53149700	-3.87053100
C	-0.00623700	1.47428000	-4.71253200
H	-1.07964400	1.45230500	-4.87313400
C	0.71869700	2.39885700	-5.35416600
H	0.18120400	3.10302300	-5.98221800
C	-0.65068600	-1.28072600	-0.40168900
C	-1.49790800	-1.41555200	-1.43192100
H	-1.78119400	-0.57753300	-2.05864100
C	-2.03757800	-2.73109500	-1.81142700
C	-0.32585200	-2.48520600	0.43510600
C	-0.87192900	-3.82250700	0.08009400
C	-1.71094500	-3.91915800	-0.96555300
O	-2.72223900	-2.87307300	-2.81867100
O	0.37213600	-2.35649800	1.42951400

C	-2.71440800	0.95210400	0.94746500
H	-3.59191300	0.49676300	0.47742200
H	-2.16453100	0.16548600	1.46374200
H	-3.08477600	1.65933800	1.69434100
C	-2.51325300	2.91452100	-0.65053400
H	-2.68534600	3.65334200	0.13776600
H	-1.88535200	3.36393300	-1.41962900
H	-3.48729200	2.68594700	-1.09272900
C	2.21180100	2.55230300	-5.33037000
H	2.69782100	1.65216300	-4.95430000
H	2.58698200	2.76281900	-6.33420700
H	2.51594400	3.38995900	-4.69502600
C	-0.46641100	-4.98197100	0.93296300
H	-0.74803300	-4.81540000	1.97439700
H	-0.92136100	-5.89720900	0.56323800
H	0.62035000	-5.09163300	0.91952000
O	-2.21531000	-5.10717800	-1.37792500
C	-3.62786300	-5.27514700	-1.14412000
H	-3.92424800	-6.14577300	-1.71846000
H	-3.79984400	-5.42749700	-0.07784600
H	-4.18069300	-4.40725500	-1.49996800
H	-2.88831900	-1.30767900	-3.99623900
O	-2.66478300	-0.47364000	-4.43616800
H	-2.26099100	-0.73575000	-5.27061300
H	-0.20988300	-3.19058400	4.48490400
O	0.19115900	-3.87034000	3.93355100
H	0.49807800	-3.39525400	3.14863500
H	-3.07539000	-4.66859900	-3.83425200
O	-3.01423800	-5.59268900	-4.11190800
H	-2.28412300	-5.91825900	-3.57338500

2

E(RM052X) = -1042.608707 a.u.

C	0.05381300	-0.01011900	-0.01020600
H	0.13970300	0.00178000	1.07895800
C	1.47669300	-0.03811100	-0.57005400
H	1.45508900	0.00289000	-1.66299200
H	2.07749900	0.79663500	-0.20398200
C	-0.77946300	1.15024000	-0.46163200
H	-0.74962400	1.34828400	-1.53234300
C	-1.52471200	1.96334200	0.29720200
C	1.99187900	-1.40076700	-0.10667400
H	2.20137700	-1.33863500	0.96814000
C	3.24061500	-1.88074500	-0.83528900
H	4.07938800	-1.20131700	-0.67036900
H	3.54257000	-2.87479800	-0.49610600
H	3.04729200	-1.93365500	-1.90962200
C	0.77935700	-2.34458100	-0.31057500
H	0.89411500	-2.78986700	-1.30338700
C	0.72794800	-3.45981300	0.69431300
H	1.68261700	-3.90050500	0.96835700
C	-0.40020900	-3.94557000	1.20660000
H	-0.37545600	-4.78623900	1.89168600
C	-1.74481600	-3.37526800	0.83635600

H	-2.43826000	-3.50802800	1.67121700
C	-0.49967100	-1.44884900	-0.35641800
C	-1.57814400	-1.84382300	0.66059900
H	-1.27726800	-1.47608700	1.64422700
C	-2.93108700	-1.22609300	0.39996700
C	-1.03472700	-1.39729400	-1.78327600
C	-2.46782600	-1.09380400	-2.03754900
C	-3.33578900	-0.97842000	-1.01520400
O	-3.71163200	-1.01954800	1.30978100
O	-0.28841800	-1.51694900	-2.74096300
C	-1.71498900	1.84134700	1.78612300
H	-1.50336700	2.79814400	2.27164200
H	-2.75554300	1.58843200	2.00998200
H	-1.08790200	1.07930800	2.24407500
C	-2.26911600	3.11942600	-0.31952700
H	-2.17567300	3.12815500	-1.40608900
H	-3.33123000	3.07944100	-0.05993600
H	-1.88700000	4.06889800	0.06723900
C	-2.32005600	-4.10504200	-0.38504900
H	-2.35402200	-5.17769000	-0.18593100
H	-3.33222100	-3.77242800	-0.62195400
H	-1.68766300	-3.95668500	-1.26401900
C	-2.85678000	-0.90228700	-3.47021800
H	-2.28490400	-0.08003200	-3.90537600
H	-2.60134500	-1.79466200	-4.04391300
H	-3.92132400	-0.70193000	-3.55632500
O	-4.64885600	-0.71266000	-1.23437900
C	-5.06930200	0.59636000	-0.83046600
H	-6.14187800	0.63096900	-1.00226100
H	-4.85572700	0.76046000	0.22370100
H	-4.57122500	1.34987700	-1.44528700

3

E(RM052X) = -1042.597937 a.u.

C	0.04085700	-0.01566400	0.10534000
H	-0.13484900	0.06407000	1.17784600
C	1.57146000	-0.13944300	-0.17787800
H	1.86744800	0.64682100	-0.87940200
H	2.15908700	0.00651400	0.72905800
C	-0.58290700	1.16045800	-0.58955700
H	-0.29196600	1.28195400	-1.63212900
C	-1.48709900	2.01682600	-0.10166800
C	1.83430900	-1.52025900	-0.82269200
H	2.02965000	-2.26182100	-0.04976700
C	2.98647600	-1.50059400	-1.81979900
H	3.92006900	-1.20969700	-1.33356500
H	3.13917100	-2.48332600	-2.27151200
H	2.78744400	-0.78488100	-2.62316400
C	0.47565400	-1.81512700	-1.46118500
H	0.38266700	-1.08882200	-2.28684200
C	0.14275800	-3.16912900	-2.01389800
H	0.94168200	-3.80212000	-2.38485300
C	-1.12475900	-3.57575800	-2.07407300
H	-1.36130700	-4.55199400	-2.48734000

C	-2.31772400	-2.77455800	-1.60105800
H	-2.77430600	-3.33126200	-0.77264400
C	-0.55199800	-1.37979400	-0.41965500
C	-1.93346200	-1.35631900	-1.08133000
H	-1.92502600	-0.66334300	-1.92459800
C	-2.99329400	-0.86790900	-0.12885400
C	-0.64095100	-2.30532100	0.78824700
C	-1.81437900	-2.10388100	1.69813700
C	-2.85374900	-1.33509600	1.29636400
O	-3.94350200	-0.19675600	-0.46759600
O	0.21260300	-3.12069400	1.07947300
C	-2.03304600	2.00068300	1.30202400
H	-1.46986700	1.35173400	1.97162800
H	-2.02422700	3.01111100	1.71949600
H	-3.07376100	1.66131600	1.28696300
C	-2.10364500	3.06844000	-0.98479100
H	-1.98205200	4.06576800	-0.55278000
H	-1.66605300	3.06502500	-1.98326600
H	-3.17798100	2.88248400	-1.07870100
C	-3.36683400	-2.65639300	-2.71295600
H	-2.93242000	-2.16516900	-3.58614700
H	-3.71946800	-3.64351600	-3.01767600
H	-4.22259900	-2.06874000	-2.37729100
C	-1.76967100	-2.85515600	3.00091600
H	-1.10450000	-3.70698100	2.87317000
H	-1.37251100	-2.25080900	3.82003300
H	-2.76074400	-3.21137200	3.27886900
O	-3.91205400	-0.97502200	2.04635500
C	-3.70122400	-0.58932700	3.40394500
H	-3.81710800	-1.43300700	4.08205200
H	-2.70893900	-0.15305800	3.52394100
H	-4.46048500	0.15841700	3.62157600

4

E(RM052X) = -1042.607228 a.u.

C	0.07432200	0.01705500	-0.03936200
H	0.16148600	0.02933200	1.04949900
C	1.49772400	0.00212200	-0.59838800
H	1.47657400	0.07122400	-1.69284800
H	2.09635000	0.83392500	-0.22105600
C	-0.72740600	1.19431700	-0.50955500
H	-0.59197400	1.46192800	-1.55548500
C	-1.52801500	1.97839700	0.22375400
C	2.01923800	-1.36406600	-0.17028800
H	2.15929500	-1.33395500	0.91511800
C	3.34732600	-1.74329700	-0.81416600
H	4.11704200	-1.02254400	-0.53058800
H	3.68474700	-2.73199500	-0.49517700
H	3.27031700	-1.74309900	-1.90351200
C	0.81509600	-2.31738500	-0.44495900
H	0.73699300	-3.00823200	0.39769200
C	0.97498800	-3.15816300	-1.68302900
H	1.91490300	-3.69212800	-1.77104300
C	0.03603000	-3.35519900	-2.60417300

H	0.21541500	-4.04191800	-3.42511800
C	-1.31690000	-2.71026100	-2.52106400
H	-1.67312000	-2.47293500	-3.52740800
C	-0.46689400	-1.42067100	-0.43531900
C	-1.16916300	-1.34932700	-1.79763500
H	-0.57065400	-0.72984700	-2.46957100
C	-2.53770800	-0.71022700	-1.75453000
C	-1.41543500	-1.82405100	0.68229900
C	-2.84433300	-1.42554500	0.61039300
C	-3.34836400	-0.86377100	-0.50700000
O	-3.02059400	-0.20750600	-2.75075300
O	-1.00604000	-2.36555800	1.69565200
C	-1.84543800	1.76101300	1.67894100
H	-2.92737500	1.66376200	1.81259000
H	-1.37969200	0.87018500	2.09668800
H	-1.53078700	2.62675500	2.26935000
C	-2.17266800	3.19787800	-0.38230200
H	-1.78177600	4.10571100	0.08744600
H	-1.98841600	3.25831400	-1.45506300
H	-3.25294700	3.19696000	-0.21462000
C	-2.31997900	-3.68337000	-1.88332700
H	-2.32414600	-4.61836600	-2.44689800
H	-2.03482300	-3.92245800	-0.85606300
H	-3.33599000	-3.28419600	-1.88383100
C	-3.66569100	-1.69211700	1.83398400
H	-3.20631100	-1.21956500	2.70390600
H	-4.68140000	-1.32921800	1.70229200
H	-3.68566800	-2.76455700	2.03781700
O	-4.66694000	-0.56011500	-0.59134000
C	-4.98983500	0.81837700	-0.81004700
H	-6.04455200	0.83908800	-1.07157700
H	-4.83115100	1.38116300	0.11312500
H	-4.39773000	1.23326800	-1.62098100

5

E(RM052X) = -1042.599086 a.u.

C	0.02159600	0.00295800	-0.04505400
H	0.07719800	0.03112400	1.04708300
C	1.45902900	-0.00571500	-0.60791900
H	1.42187000	0.15655900	-1.68836600
H	2.06149500	0.79383300	-0.17427800
C	-0.81421900	1.14540300	-0.53774800
H	-0.71264800	1.36653100	-1.59936700
C	-1.63637100	1.92107400	0.18018700
C	2.03451400	-1.41545200	-0.31695300
H	2.65282000	-1.35716800	0.58264500
C	2.91795000	-1.95260800	-1.43970400
H	3.72303200	-1.24296500	-1.64606500
H	3.38222100	-2.90021400	-1.15665000
H	2.33968500	-2.10050400	-2.34875800
C	0.77482100	-2.25028100	0.04629200
H	0.72559600	-2.22129000	1.14295800
C	0.60316400	-3.69087500	-0.34088600
H	1.45493400	-4.27861700	-0.66211500

C	-0.61125400	-4.23459100	-0.26016600
H	-0.75947000	-5.27821300	-0.52080400
C	-1.86117500	-3.50113000	0.18023800
H	-2.59888800	-3.63470500	-0.61992100
C	-0.45837600	-1.44201700	-0.38786500
C	-1.65874100	-1.96174500	0.39982500
H	-1.49723300	-1.77218500	1.46476200
C	-2.94560300	-1.27645500	0.01741000
C	-0.76186000	-1.52331200	-1.87788800
C	-2.15064900	-1.22700200	-2.33747000
C	-3.14920900	-1.05510300	-1.44954500
O	-3.81566500	-1.00685800	0.82208700
O	0.09717100	-1.72263600	-2.71705000
C	-1.93736300	1.74949800	1.64536000
H	-1.31311400	1.00251800	2.13160500
H	-1.81126900	2.69999800	2.17113400
H	-2.97858200	1.43977000	1.77502700
C	-2.36024900	3.07604900	-0.46240000
H	-3.43751800	3.00924800	-0.28388600
H	-2.02746400	4.02245200	-0.02552200
H	-2.18600800	3.11531700	-1.53831000
C	-2.44986600	-4.12594800	1.45088900
H	-3.35167000	-3.59027800	1.75389100
H	-2.70499200	-5.17437900	1.28680100
H	-1.72431200	-4.07440400	2.26547600
C	-2.33791800	-1.08854400	-3.81626300
H	-2.01768800	-2.00474100	-4.31478500
H	-3.37843700	-0.88390700	-4.05357000
H	-1.70266600	-0.28794300	-4.20113200
O	-4.41253900	-0.76510900	-1.85381100
C	-4.84489500	0.56377900	-1.53595000
H	-5.87243500	0.63339600	-1.88318000
H	-4.80047300	0.73503600	-0.46242500
H	-4.22402600	1.29067800	-2.06498900

2w

E(RM052X) = -1271.839265 a.u.

C	-0.00309900	-0.03240100	-0.02506600
H	0.06608400	-0.01577600	1.06495500
C	1.42426900	-0.04649700	-0.57333600
H	1.40640200	0.01019000	-1.66623100
H	2.00984000	0.79493600	-0.19824800
C	-0.83053400	1.12358400	-0.50101500
H	-0.77018000	1.32105500	-1.57077200
C	-1.57016200	1.95059900	0.25012400
C	1.95597500	-1.40273600	-0.11166900
H	2.15860200	-1.33923400	0.96393400
C	3.21518100	-1.86429200	-0.83424500
H	4.04298300	-1.17289800	-0.66427900
H	3.53027700	-2.85415500	-0.49505600
H	3.02899700	-1.91939100	-1.90997600
C	0.75885100	-2.36427500	-0.32232500
H	0.88348400	-2.80742800	-1.31486400
C	0.71803500	-3.48486900	0.67753500

H	1.67689600	-3.91961600	0.94566200
C	-0.40443700	-3.98362200	1.18911100
H	-0.37012000	-4.83108400	1.86539500
C	-1.75728500	-3.42855100	0.82601800
H	-2.44453800	-3.56973400	1.66620100
C	-0.53247800	-1.48834500	-0.36809700
C	-1.59563900	-1.89196800	0.65922100
H	-1.28484800	-1.53217100	1.64177600
C	-2.94080100	-1.27601300	0.40599200
C	-1.07433800	-1.44196300	-1.78382200
C	-2.51020800	-1.13579700	-2.03257500
C	-3.36041200	-1.02664600	-0.99590000
O	-3.72392300	-1.04701700	1.32149400
O	-0.33024400	-1.56196900	-2.74876800
C	-1.78418900	1.84084400	1.73655400
H	-1.47094100	2.76622600	2.22913700
H	-2.85137000	1.71903200	1.95036500
H	-1.26700700	1.00888300	2.20895500
C	-2.25933300	3.13237300	-0.38427000
H	-2.13888700	3.13552100	-1.46823400
H	-3.32749000	3.13913200	-0.14639000
H	-1.84765300	4.06593200	0.01125900
C	-2.33990000	-4.16187300	-0.38888900
H	-2.32062200	-5.23725300	-0.20199300
H	-3.37520400	-3.87236200	-0.57275700
H	-1.73593500	-3.97976500	-1.28222700
C	-2.92022900	-0.91604000	-3.45397600
H	-2.44163600	-0.01556600	-3.84698700
H	-2.57940800	-1.75268500	-4.06566600
H	-4.00043800	-0.82143200	-3.52942500
O	-4.67246300	-0.70483400	-1.18624300
C	-4.96127200	0.67921200	-0.92782000
H	-6.02481000	0.80388900	-1.11192100
H	-4.72609600	0.92552400	0.10677100
H	-4.38402900	1.30646400	-1.60914900
H	0.57613800	1.29502000	-4.36511200
O	-0.25203500	1.00405600	-3.96941300
H	-0.14954200	0.05217400	-3.82086300
H	-2.14355200	-1.70166900	4.16845500
O	-2.12823000	-0.84366000	3.73073400
H	-2.83165500	-0.89173600	3.06316300
O	-5.56135900	-3.06416800	0.22194500
H	-5.65628700	-2.38577800	-0.45962500
H	-5.28288700	-2.54611300	0.98722000

3w

E(RM052X) = -1271.831450 a.u.

C	0.03406700	0.01599300	-0.00593200
H	0.01521200	0.05786500	1.08333600
C	1.51575700	0.00215900	-0.48437800
H	1.60754500	0.63524300	-1.37359300
H	2.18621500	0.40985500	0.27296400
C	-0.77178700	1.15009800	-0.56444100
H	-0.75896000	1.23410900	-1.64974500

C	-1.54355200	2.01472800	0.10692800
C	1.86093200	-1.44741700	-0.87778000
H	2.07964300	-2.03686400	0.01284400
C	3.02119000	-1.54087700	-1.86039500
H	3.93439500	-1.12701500	-1.42796200
H	3.22460300	-2.57708200	-2.13947800
H	2.79621000	-0.98114100	-2.77292400
C	0.51926400	-1.88849400	-1.46379400
H	0.39035400	-1.25721700	-2.35911800
C	0.22937700	-3.30184600	-1.87484400
H	1.04679900	-3.96436400	-2.13714700
C	-1.03365600	-3.72125500	-1.94630100
H	-1.25217900	-4.73840800	-2.25717900
C	-2.24866000	-2.88072300	-1.61382200
H	-2.76533500	-3.38048900	-0.78515300
C	-0.52823400	-1.39077800	-0.46966200
C	-1.88818000	-1.42498200	-1.17139500
H	-1.86459300	-0.79010300	-2.05734100
C	-2.97318000	-0.90708700	-0.27712900
C	-0.63725500	-2.22900300	0.79008600
C	-1.84268500	-2.01772500	1.64628200
C	-2.88753200	-1.29752600	1.16831300
O	-3.93770300	-0.27416300	-0.68254900
O	0.24629200	-2.98211700	1.16886200
C	-1.71812800	2.06793500	1.60100200
H	-1.15612300	1.30332000	2.13605700
H	-1.40049300	3.04599500	1.97523300
H	-2.78113100	1.96714300	1.83823700
C	-2.37239900	3.03204200	-0.63188400
H	-2.09926200	4.04805900	-0.33097800
H	-2.26809500	2.93441000	-1.71177100
H	-3.42385700	2.89071100	-0.36391900
C	-3.21777100	-2.82910800	-2.80137500
H	-2.72887700	-2.36742800	-3.66179700
H	-3.53699400	-3.83346500	-3.08476900
H	-4.10503300	-2.24413600	-2.55024800
C	-1.81453900	-2.67882600	2.99473900
H	-1.39760300	-3.68117000	2.89005800
H	-1.17650700	-2.13283600	3.69508300
H	-2.81309600	-2.76156700	3.41476300
O	-3.99078200	-0.93497100	1.84045300
C	-3.90367800	-0.44550200	3.18819200
H	-4.27062000	-1.20057200	3.88042800
H	-2.87477300	-0.18228900	3.42929600
H	-4.53736600	0.43679900	3.21612900
H	-3.46079800	0.63623300	-2.37435000
O	-3.01677500	0.88820500	-3.20020200
H	-3.55396900	0.49605200	-3.89731300
H	0.52128400	-5.52479200	3.11562600
O	-0.09693100	-5.59052000	2.37994400
H	0.10987800	-4.81722900	1.83378600
H	-4.89127200	0.79229900	0.75646800
O	-5.17174000	1.59339700	1.22878600
H	-5.70732400	2.08194000	0.59515200

4w

E(RM052X) = -1271.839078 a.u.

C	-0.04518600	-0.05280600	-0.00074400
H	-0.07840600	-0.04157300	1.09147000
C	1.42781000	-0.06522800	-0.42118200
H	1.50688100	0.06657200	-1.50751800
H	1.99271800	0.73637400	0.05880800
C	-0.78810200	1.11848500	-0.56966700
H	-0.63099900	1.29735900	-1.63045000
C	-1.54026200	2.01255400	0.08903100
C	1.89368100	-1.46153700	-0.03255400
H	1.86792500	-1.52297300	1.06136000
C	3.29994600	-1.80798900	-0.50547700
H	4.03017600	-1.16402500	-0.01167100
H	3.55902900	-2.84442100	-0.27592300
H	3.40094500	-1.66030600	-1.58265900
C	0.74889200	-2.37263500	-0.55007900
H	0.62992900	-3.19805700	0.15590100
C	1.00017000	-2.99695400	-1.89802200
H	1.99266000	-3.40044300	-2.06405100
C	0.06006200	-3.18524000	-2.82052700
H	0.28614200	-3.73137200	-3.73019100
C	-1.34959900	-2.70142200	-2.62242800
H	-1.78964800	-2.44940800	-3.59151400
C	-0.54440600	-1.49612600	-0.48357700
C	-1.26979800	-1.37282100	-1.82829600
H	-0.71679200	-0.68542400	-2.47203800
C	-2.65706600	-0.80185100	-1.71957500
C	-1.45698100	-1.97131200	0.62253500
C	-2.86609500	-1.50004100	0.65445500
C	-3.40389600	-0.92741800	-0.44015400
O	-3.21841600	-0.32928400	-2.70301700
O	-1.03654300	-2.63266600	1.56384100
C	-1.84117400	1.98551300	1.56310500
H	-2.92281200	2.02284200	1.72902900
H	-1.44859900	1.11542100	2.08553500
H	-1.43028700	2.88335700	2.03664000
C	-2.10767600	3.19574100	-0.65469100
H	-1.63827700	4.12114300	-0.30603400
H	-1.94469400	3.10592900	-1.72958800
H	-3.18010600	3.30207200	-0.46495800
C	-2.21873100	-3.78650700	-1.97162400
H	-2.14686700	-4.70538700	-2.55677500
H	-1.86347900	-4.01868500	-0.96410000
H	-3.27044500	-3.49544000	-1.93660700
C	-3.61871600	-1.71353500	1.92947000
H	-3.11520000	-1.19243800	2.74711700
H	-4.64133200	-1.35840300	1.83672100
H	-3.62020500	-2.77623200	2.17824200
O	-4.71142700	-0.54579300	-0.45428200
C	-4.94238700	0.86684700	-0.58800800
H	-6.01332300	0.97918800	-0.73377200
H	-4.63628900	1.37098700	0.32903200
H	-4.40176200	1.26532000	-1.44283500
H	-0.80886400	-1.52287100	3.12055900

O	-0.79267400	-0.65290600	3.54692800
H	-0.07308500	-0.68764300	4.18575800
H	-0.99838700	1.21112600	-4.79626200
O	-1.23213400	1.35749100	-3.87364600
H	-2.00200100	0.79046600	-3.70721200
O	-5.34460500	-2.37407700	-2.60858700
H	-5.53665000	-1.91409800	-1.78105100
H	-4.85248700	-1.70784300	-3.10463500

5w

E(RM052X) = -1271.830886 a.u.

C	-0.01311500	-0.01343400	-0.03558200
H	0.00486700	0.01124100	1.05778600
C	1.43904900	-0.01992200	-0.56098400
H	1.42433200	0.18274600	-1.63469600
H	2.03244700	0.76472700	-0.08897000
C	-0.82285500	1.13286100	-0.56576700
H	-0.66729800	1.35158900	-1.62159100
C	-1.66007300	1.91869600	0.12346000
C	2.00409500	-1.43849700	-0.29502200
H	2.61097700	-1.40366100	0.61317800
C	2.90306800	-1.95429000	-1.41567800
H	3.71132600	-1.24124500	-1.59731400
H	3.36328300	-2.90725300	-1.14498500
H	2.33952700	-2.08835900	-2.33621900
C	0.73895000	-2.27813100	0.03353300
H	0.67476100	-2.27427200	1.12915200
C	0.55907100	-3.70651900	-0.39687500
H	1.40252000	-4.28535000	-0.75414500
C	-0.65891500	-4.24390100	-0.31751500
H	-0.81890600	-5.27637400	-0.61267500
C	-1.89386000	-3.52455700	0.18197400
H	-2.68445600	-3.67150800	-0.56020200
C	-0.48848000	-1.45856900	-0.39617400
C	-1.68554100	-1.97990500	0.39550900
H	-1.51315100	-1.78608100	1.45620600
C	-2.96156400	-1.29994600	0.00191500
C	-0.78191100	-1.51515300	-1.88312100
C	-2.17244200	-1.24132700	-2.35347800
C	-3.16602800	-1.09296600	-1.45879200
O	-3.84375300	-0.99414200	0.79418200
O	0.09375300	-1.67626900	-2.72005800
C	-2.01394600	1.75857000	1.57896600
H	-1.60010000	0.86496800	2.04197800
H	-1.68437000	2.63496800	2.14591500
H	-3.10255600	1.70364800	1.68442800
C	-2.32381900	3.09546600	-0.54537400
H	-3.41193000	3.04769100	-0.43810400
H	-2.00493600	4.02970100	-0.07271500
H	-2.07715400	3.14703300	-1.60634600
C	-2.39797400	-4.14651300	1.49046300
H	-3.28847200	-3.62261100	1.84401500
H	-2.65252400	-5.19735400	1.34409500
H	-1.63647700	-4.07220300	2.26885000

C	-2.37402800	-1.09122100	-3.82843700
H	-1.91390600	-1.93399500	-4.34582100
H	-3.43412600	-1.04746700	-4.06496000
H	-1.87967100	-0.18451200	-4.18544200
O	-4.43980500	-0.79469700	-1.85158600
C	-4.78129100	0.58998700	-1.67700700
H	-5.79103400	0.70119700	-2.06285700
H	-4.74785300	0.85426200	-0.62127300
H	-4.08964300	1.21244600	-2.24737200
O	0.27732400	0.87940200	-3.96292000
H	0.37764900	-0.06980500	-3.79501700
H	1.16123400	1.19731100	-4.17540600
H	-2.87711900	-0.45273400	3.99499800
O	-2.61088800	-1.15518200	3.39228100
H	-3.20131300	-1.07109000	2.62545500
H	-5.28121800	-2.50115700	-1.13735800
O	-5.15523000	-3.29258100	-0.59504000
H	-5.20580700	-2.95161100	0.30533000

TS1n

E(RM052X) = -1042.517296 a.u.

1 imaginary frequency -376.255 cm⁻¹

C	0.13968200	0.01631200	0.05149100
H	0.16089900	0.13640200	1.13717000
C	1.61328500	-0.14525700	-0.42750200
H	1.95128600	0.81376200	-0.83066600
H	2.25174800	-0.38600800	0.41866200
C	-0.48667300	1.24201600	-0.57164600
H	-0.08811600	1.53312800	-1.54222000
C	-1.45169800	2.00748200	-0.05011600
C	1.76723700	-1.24541600	-1.50771100
H	2.15807200	-2.15253900	-1.04306200
C	2.72198000	-0.80680400	-2.62497600
H	3.69574500	-0.53975600	-2.20903400
H	2.86532900	-1.60319800	-3.35691600
H	2.32564600	0.06918200	-3.14548400
C	0.40006400	-1.52927200	-2.04871200
H	-0.12038000	-0.64287600	-2.38064600
C	-0.07124000	-2.75137600	-2.50350000
H	0.54385600	-3.63559600	-2.36552300
C	-1.43326600	-2.91785600	-2.79234500
H	-1.81795000	-3.93285900	-2.76806000
C	-2.35740400	-1.88142000	-2.79485000
H	-3.39881200	-2.18349000	-2.74330400
C	-0.67630200	-1.25964100	-0.21207300
C	-2.03685000	-1.25164300	-0.52477400
H	-2.54991500	-0.31276000	-0.68167300
C	-2.92159800	-2.36123200	-0.16561300
C	-0.15551600	-2.46742900	0.50335500
C	-0.94857300	-3.71194800	0.47418200
C	-2.25473900	-3.66732700	0.13364100
O	-4.13799400	-2.24446200	-0.10722400
O	0.91782500	-2.42990800	1.09155500
C	-2.11778900	1.74192000	1.27307000

H	-1.70896100	0.87469700	1.78780600
H	-2.02420100	2.61369600	1.92710000
H	-3.18820400	1.56893200	1.12484200
C	-1.96668800	3.21810100	-0.78376900
H	-1.83222700	4.12011400	-0.17952900
H	-1.45414000	3.36142700	-1.73542800
H	-3.03930000	3.12406000	-0.97779400
C	-2.15489400	-0.51934600	-3.43421400
H	-2.03554500	0.29934500	-2.72248100
H	-1.28830500	-0.52836300	-4.09673500
H	-3.03387000	-0.29193900	-4.04001400
C	-0.29994900	-4.98844500	0.92183900
H	0.75997800	-4.82043700	1.09659800
H	-0.75502100	-5.35005500	1.84647200
H	-0.43761000	-5.76831800	0.17053900
O	-2.96468200	-4.80775500	0.20690200
C	-4.20893200	-4.94790600	-0.48894000
H	-4.35449800	-6.02137300	-0.58606700
H	-5.02008000	-4.49541400	0.07193400
H	-4.15691300	-4.49251900	-1.47814300

TS1x

E(RM052X) = -1042.506665 a.u.

1 imaginary frequency -396.724 cm⁻¹

C	-0.02706600	-0.02897100	0.08303700
H	-0.11269600	0.04168200	1.16735100
C	1.49362600	-0.13105300	-0.25043100
H	1.74133100	0.64888600	-0.97848200
H	2.08812000	0.07899100	0.64043500
C	-0.60279300	1.20984900	-0.55002000
H	-0.43264800	1.29109200	-1.62261900
C	-1.26576100	2.20655500	0.04427300
C	1.89745100	-1.49438000	-0.83619300
H	1.98772100	-2.20552500	-0.01730600
C	3.24630800	-1.41614900	-1.56043300
H	4.02070700	-1.06267000	-0.87616600
H	3.54661100	-2.39383500	-1.94030100
H	3.19997100	-0.72397100	-2.40395600
C	0.76994800	-1.94523300	-1.72937400
H	0.45280200	-2.97555600	-1.65745500
C	0.39828000	-1.17365200	-2.81705900
H	0.99040200	-0.28204000	-3.00597700
C	-0.85044100	-1.21079200	-3.45343700
H	-1.10509200	-0.32489400	-4.02765900
C	-1.89738200	-2.06591900	-3.16295400
H	-2.87096200	-1.74614400	-3.52320700
C	-0.82336300	-1.29193100	-0.28681000
C	-2.05871000	-1.24175300	-0.92994000
H	-2.42806900	-0.30101300	-1.31375000
C	-3.11998900	-2.22669000	-0.68647400
C	-0.62379700	-2.41716100	0.67729600
C	-1.55273500	-3.57693200	0.67623100
C	-2.75264500	-3.46516200	0.07412100
O	-4.25545900	-2.07377800	-1.11375300

O	0.27890200	-2.38128700	1.50237000
C	-1.61164700	2.27029000	1.50818600
H	-2.69580500	2.35136200	1.63000700
H	-1.27404500	1.40304400	2.07099900
H	-1.17510800	3.16563700	1.96051400
C	-1.74083300	3.39585900	-0.75048200
H	-1.30567400	4.31989800	-0.35802700
H	-1.47358300	3.31015200	-1.80402000
H	-2.82733800	3.50082600	-0.67632100
C	-1.82157800	-3.55192600	-2.91869500
H	-1.54283900	-4.03734500	-3.85874800
H	-1.09870600	-3.85318700	-2.16683100
H	-2.79450700	-3.94157500	-2.61970000
C	-1.12147500	-4.78568300	1.44911900
H	-0.81502200	-4.48895500	2.45233800
H	-1.92652100	-5.51372900	1.50119600
H	-0.25221800	-5.25025700	0.97713300
O	-3.59756500	-4.51909800	0.04951700
C	-5.00069200	-4.31278700	0.28019200
H	-5.35326000	-5.23557500	0.73672800
H	-5.16223900	-3.47748600	0.95960900
H	-5.51990000	-4.12305100	-0.65366400

TS2n

E(RM052X) = -1042.513860 a.u.

1 imaginary frequency -390.018 cm⁻¹

C	-0.01223100	0.00794800	0.01739700
H	0.00241800	-0.02703400	1.10938800
C	1.44253000	-0.08018300	-0.49884200
H	1.46997900	0.27603700	-1.52634000
H	2.06657000	0.58765300	0.09800200
C	-0.66175900	1.29134800	-0.43293800
H	-0.63581700	1.44710600	-1.50739700
C	-1.25153800	2.21854000	0.32745600
C	1.98526100	-1.54066300	-0.45888800
H	2.77417100	-1.58469300	0.30119200
C	2.59062900	-1.98711600	-1.78848700
H	3.38076500	-1.29473800	-2.08488900
H	3.03084100	-2.98339300	-1.70557300
H	1.83917700	-1.99305700	-2.57777500
C	0.88020200	-2.42286000	0.05504800
H	0.61283100	-2.17649400	1.06979100
C	0.48122400	-3.67414500	-0.39315800
H	0.87279700	-4.06339600	-1.32650900
C	-0.65063400	-4.27696800	0.17284800
H	-1.15453400	-5.03362100	-0.42004100
C	-1.32560800	-3.76631200	1.27778400
H	-2.32396300	-4.16198200	1.43604600
C	-0.83477600	-1.20315000	-0.42751800
C	-1.88369400	-1.69149000	0.35815000
H	-2.07863500	-1.24243000	1.32557100
C	-3.05554700	-2.33943600	-0.23645900
C	-0.93160900	-1.44646600	-1.89860800
C	-1.86182300	-2.47787100	-2.39762400

C	-2.86799600	-2.91332400	-1.60890700
O	-4.12864900	-2.42935000	0.34061900
O	-0.24785600	-0.82049400	-2.70013000
C	-1.40215500	2.16452700	1.82514900
H	-2.46306600	2.15044100	2.09267600
H	-0.92944000	1.29691100	2.28150000
H	-0.97407000	3.06269100	2.27980900
C	-1.85551900	3.44856700	-0.30048100
H	-2.92410300	3.51201800	-0.07358100
H	-1.39128600	4.35476000	0.10044200
H	-1.73268100	3.44762000	-1.38335900
C	-0.66438400	-3.30074200	2.56593500
H	-0.75936800	-2.23262100	2.76731200
H	-1.14065300	-3.82064300	3.39922700
H	0.39418900	-3.56116500	2.57590900
C	-1.69335400	-2.89639500	-3.82669600
H	-0.65521100	-3.17744100	-4.01460100
H	-2.35043200	-3.72894600	-4.06418200
H	-1.91752800	-2.05993300	-4.49132300
O	-3.78258200	-3.76224000	-2.11362800
C	-4.51745200	-4.63460800	-1.24716000
H	-4.81469200	-5.47132000	-1.87522100
H	-3.88900700	-4.99588600	-0.43219700
H	-5.38602000	-4.13005400	-0.83710700

TS2x

E(RM052X) = -1042.509004 a.u.

1 imaginary frequency -402.932 cm⁻¹

C	0.06144000	0.02421500	0.01235900
H	0.05781800	0.01282200	1.10445200
C	1.51376000	-0.07068600	-0.47415100
H	1.53844900	0.09705000	-1.54894900
H	2.09889600	0.72286800	-0.00297600
C	-0.57512400	1.29396200	-0.49860600
H	-0.49934000	1.42443100	-1.57624100
C	-1.21426300	2.23592300	0.20084300
C	2.13616900	-1.46216400	-0.16674100
H	2.75309200	-1.36010200	0.73135300
C	3.01786400	-1.93530700	-1.32353600
H	3.80172400	-1.20316200	-1.52846800
H	3.49396700	-2.89118300	-1.09577300
H	2.41238500	-2.04561300	-2.22466500
C	1.04541700	-2.44904000	0.16836100
H	0.71520300	-3.11582400	-0.61468000
C	0.75723000	-2.69566900	1.50197300
H	1.38645800	-2.19222900	2.23089600
C	-0.43890200	-3.23194000	1.99085400
H	-0.65455400	-3.05376000	3.03944000
C	-1.48684300	-3.66794900	1.19485800
H	-2.43617600	-3.81159400	1.70068000
C	-0.79613200	-1.17403500	-0.40992800
C	-1.87007000	-1.56909500	0.38425100
H	-1.97650700	-1.14571400	1.37525200
C	-3.16873100	-1.97582100	-0.17879500

C	-0.90940500	-1.45280500	-1.87505400
C	-2.15818900	-2.03481100	-2.43502300
C	-3.21924200	-2.29169700	-1.64115700
O	-4.17706600	-2.02534600	0.50834000
O	0.00513300	-1.20061600	-2.65037000
C	-1.43555400	2.21885200	1.69037300
H	-1.05485800	3.14094500	2.13926900
H	-2.50724900	2.18012700	1.90810900
H	-0.95986400	1.37719500	2.18954300
C	-1.80371200	3.43822600	-0.49116200
H	-1.63338600	3.40675300	-1.56728900
H	-2.88191000	3.49478200	-0.31301000
H	-1.36825900	4.36215300	-0.09873600
C	-1.30632800	-4.48008000	-0.06732600
H	-0.47732500	-5.18011700	0.05894000
H	-2.20981500	-5.05344200	-0.27836200
H	-1.09863700	-3.88016000	-0.95173500
C	-2.15965500	-2.29356500	-3.91118400
H	-1.28308300	-2.88048000	-4.18833700
H	-3.06613700	-2.81394600	-4.20806700
H	-2.09028700	-1.35127400	-4.45832800
O	-4.36384900	-2.74458200	-2.18758200
C	-5.23729700	-3.60629200	-1.44632400
H	-5.76135600	-4.19185000	-2.19853800
H	-4.67049000	-4.26970700	-0.79323800
H	-5.93671900	-3.02723200	-0.85228000

TS1nw

E(RM052X) = -1271.752046 a.u.

1 imaginary frequency -344.881 cm⁻¹

C	-0.01903000	0.00967900	-0.01238000
H	-0.00202800	0.10666400	1.07598800
C	1.45426300	-0.06033100	-0.50925200
H	1.73168100	0.92089900	-0.90356100
H	2.12194100	-0.27425100	0.32214600
C	-0.73575600	1.19846200	-0.61047300
H	-0.35772300	1.54403600	-1.57089400
C	-1.78548800	1.84459800	-0.09108700
C	1.64571500	-1.13514800	-1.60839300
H	2.09158600	-2.02938800	-1.16778800
C	2.55562500	-0.63564600	-2.73733100
H	3.52381000	-0.33055700	-2.33525500
H	2.72109100	-1.41294000	-3.48479500
H	2.10853700	0.22880000	-3.23487900
C	0.28360000	-1.47958400	-2.13080700
H	-0.27961700	-0.61800100	-2.45547400
C	-0.12041200	-2.71541100	-2.62068200
H	0.55457800	-3.56101100	-2.51837300
C	-1.45978600	-2.97419700	-2.93595800
H	-1.75163400	-4.01937800	-2.97652400
C	-2.51890500	-2.07475500	-2.91322800
H	-3.48256200	-2.57602400	-2.88328900
C	-0.75957000	-1.30829300	-0.30519500
C	-2.13020600	-1.34804000	-0.58124000

H	-2.65907900	-0.42297400	-0.75963200
C	-2.94272100	-2.50521000	-0.28983000
C	-0.17770900	-2.50856600	0.35518400
C	-0.90354800	-3.80188100	0.27502100
C	-2.22100600	-3.77822500	0.00306900
O	-4.18526600	-2.48447000	-0.27169200
O	0.88415200	-2.44343400	0.96700100
C	-2.44809800	1.48172200	1.21005900
H	-3.47004800	1.14700500	1.00756300
H	-1.92687800	0.69148200	1.74842000
H	-2.51286600	2.36055200	1.85805900
C	-2.44691000	2.97606500	-0.83022600
H	-2.47886600	3.87899900	-0.21384600
H	-1.92907200	3.20868300	-1.76136600
H	-3.47947500	2.69949000	-1.06090300
C	-2.63859300	-0.65907800	-3.41398600
H	-1.73546400	-0.05905900	-3.37821900
H	-2.94729900	-0.72661500	-4.46332700
H	-3.43058800	-0.13948600	-2.87344000
C	-0.14362100	-5.04645800	0.61491100
H	0.19402400	-5.02340700	1.65311300
H	-0.76081000	-5.92532700	0.44436100
H	0.75582500	-5.11237500	-0.00194200
O	-2.95558000	-4.92873800	-0.04055400
C	-3.76732500	-5.15483200	1.12476500
H	-4.32803700	-6.06438500	0.92661400
H	-3.12397600	-5.29641900	1.99525100
H	-4.44546800	-4.31859000	1.27928000
H	-4.80910300	-0.73871500	-0.63554000
O	-4.90806700	0.20049200	-0.88236200
H	-5.81879100	0.29482200	-1.18055800
H	1.46755100	-3.60726000	3.85392700
O	1.80528300	-4.14589400	3.13094700
H	1.68322500	-3.59099500	2.34546800
H	-4.91731100	-3.82604200	-1.61111700
O	-4.69816400	-4.47676900	-2.29413700
H	-4.05691600	-5.03091500	-1.83054400

TS1xw

E(RM052X) = -1271.739294 a.u.

1 imaginary frequency -357.686 cm⁻¹

C	-0.08445500	-0.02274700	0.02133000
H	-0.12647700	0.03476000	1.10743300
C	1.42361000	-0.05888600	-0.37805100
H	1.59322400	0.70259200	-1.14568100
H	2.03690500	0.22377200	0.47933000
C	-0.73884900	1.20683800	-0.54740400
H	-0.91659800	1.19405900	-1.62149100
C	-1.06480800	2.31425500	0.12534300
C	1.86216800	-1.42171000	-0.93481000
H	1.99502400	-2.11652200	-0.10621200
C	3.19269000	-1.31859700	-1.69060500
H	3.96860300	-0.92646600	-1.03011900
H	3.51544500	-2.29379900	-2.05828000

H	3.10358500	-0.64514600	-2.54561600
C	0.73519700	-1.92656800	-1.79886600
H	0.48327000	-2.97657300	-1.74571100
C	0.29988400	-1.16384100	-2.87489800
H	0.83516200	-0.23745500	-3.06290900
C	-0.95078800	-1.27298100	-3.49099700
H	-1.28727100	-0.40441600	-4.04828900
C	-1.92741200	-2.20924200	-3.19892900
H	-2.92015800	-1.94547800	-3.54748100
C	-0.84750600	-1.30941900	-0.33491000
C	-2.09654800	-1.29288000	-0.96598100
H	-2.47891100	-0.37525900	-1.39099200
C	-3.11697300	-2.29710400	-0.72028000
C	-0.61830300	-2.42043300	0.62679700
C	-1.53145900	-3.60074200	0.65864900
C	-2.73836300	-3.50257400	0.07852500
O	-4.26961000	-2.19884400	-1.16028100
O	0.28326100	-2.38651100	1.45957200
C	-0.84523400	2.52473500	1.60220100
H	-1.80371700	2.52618100	2.13136300
H	-0.19310500	1.78097100	2.05781000
H	-0.39567400	3.50805800	1.76696100
C	-1.70071800	3.48312500	-0.58175400
H	-1.06131900	4.36868800	-0.51796800
H	-1.88993300	3.26441000	-1.63290200
H	-2.65174100	3.74456900	-0.10776400
C	-1.73075900	-3.67945500	-2.93169000
H	-1.22243500	-4.12439800	-3.79195100
H	-1.13261900	-3.90320700	-2.05152800
H	-2.69921600	-4.16817200	-2.82339300
C	-1.07963400	-4.78847100	1.44982300
H	-0.91751700	-4.50262000	2.49006100
H	-1.81567700	-5.58629500	1.39422000
H	-0.12187900	-5.15018100	1.07104300
O	-3.62522200	-4.53627500	0.10698800
C	-4.80659500	-4.30561200	0.89647700
H	-5.47148800	-5.13882900	0.68659800
H	-4.53894500	-4.29369400	1.95424000
H	-5.28086000	-3.37120700	0.60777400
H	1.22289600	-0.95394300	2.39871200
O	1.48415300	-0.16264500	2.89535300
H	1.18708600	-0.32931800	3.79600700
H	-4.97110400	0.52384300	-3.13827700
O	-4.17456400	-0.00464000	-3.02304200
H	-4.41459000	-0.70185400	-2.38921300
O	-5.06403100	-4.77351900	-2.36478400
H	-4.49800200	-5.18380500	-1.69980200
H	-5.06664100	-3.84876500	-2.07849700

TS2nw

E(RM052X) = -1271.746151 a.u.

1 imaginary frequency -364.055 cm⁻¹

C	-0.10118100	-0.04979300	0.06575800
H	-0.08579100	-0.09778000	1.15729900

C	1.35378200	-0.03592700	-0.45229300
H	1.36130000	0.34606800	-1.47104500
H	1.93908900	0.65298600	0.16009200
C	-0.86032600	1.17862900	-0.37277700
H	-1.20785500	1.16324000	-1.40195100
C	-1.12928200	2.26284000	0.35972000
C	1.96399400	-1.46715100	-0.43945000
H	2.72196200	-1.50535400	0.35113100
C	2.64671800	-1.82656700	-1.75801900
H	3.41052700	-1.08180300	-1.98951900
H	3.13546700	-2.80133000	-1.69792900
H	1.93082500	-1.83718400	-2.57974300
C	0.88503200	-2.42770500	-0.00112200
H	0.62578200	-2.29900600	1.03746100
C	0.57097400	-3.66823700	-0.55733700
H	0.98162100	-3.93172700	-1.52637900
C	-0.49263100	-4.42512300	-0.05657500
H	-0.93607000	-5.15412500	-0.72800900
C	-1.21358400	-4.15265100	1.10200100
H	-2.17441000	-4.65787500	1.13713700
C	-0.83682400	-1.31422800	-0.38615600
C	-1.84602200	-1.86063800	0.42080000
H	-1.95628600	-1.52122700	1.44408500
C	-2.99044100	-2.54345200	-0.12966100
C	-0.95935200	-1.51215300	-1.85808800
C	-1.95415600	-2.46941900	-2.39072800
C	-2.91896800	-2.92661200	-1.57297800
O	-4.01490100	-2.81371400	0.51666200
O	-0.27019900	-0.87669600	-2.65403000
C	-0.70861900	2.47680900	1.78959700
H	-1.58650500	2.62231700	2.42631300
H	-0.12372000	1.65470800	2.19804100
H	-0.10845800	3.38811000	1.86881700
C	-1.90622000	3.40849000	-0.23631000
H	-2.80926300	3.60681100	0.34917000
H	-1.31289700	4.32793800	-0.22501700
H	-2.20257100	3.19652200	-1.26376400
C	-0.69760900	-3.79012200	2.47158200
H	-1.34385600	-3.06958200	2.97378300
H	-0.74524500	-4.71139000	3.06177600
H	0.33557600	-3.45354000	2.49006000
C	-1.90267300	-2.76106300	-3.85894300
H	-2.18807300	-1.86476700	-4.41465900
H	-0.88607600	-3.02151900	-4.15694000
H	-2.57963400	-3.57448000	-4.10855900
O	-3.88956300	-3.76660200	-2.03441200
C	-5.14927800	-3.11778700	-2.28965900
H	-5.81798600	-3.89623500	-2.64678400
H	-5.53544900	-2.67684600	-1.37368900
H	-5.01598000	-2.35491200	-3.05835400
O	-2.30829600	0.65963400	-3.87516700
H	-1.45709600	0.23644300	-3.68806200
H	-2.10545500	1.37673200	-4.48502600
H	-3.95278800	-1.23960100	3.35837200
O	-3.45439400	-2.04845600	3.20088800
H	-3.79001200	-2.38230300	2.34874300

H	-3.91204100	-5.44470900	-0.80822700
O	-3.98208600	-5.68202800	0.12586800
H	-4.34978800	-4.87002100	0.50290400

TS2xw

E(RM052X) = -1271.743739 a.u.

1 imaginary frequency -353.411 cm⁻¹

C	0.05595200	0.03597400	-0.03123200
H	0.06815500	0.01968400	1.06088300
C	1.50512800	0.00091600	-0.53021700
H	1.51189400	0.12272500	-1.61151700
H	2.05408200	0.84246900	-0.10029800
C	-0.63817700	1.28296100	-0.52363800
H	-0.53124800	1.46135300	-1.59179300
C	-1.36301100	2.15262800	0.18627600
C	2.19638400	-1.33820700	-0.16193800
H	2.73793000	-1.18291200	0.77613700
C	3.19313200	-1.75251400	-1.24552000
H	3.92033000	-0.95771900	-1.42380100
H	3.73370700	-2.65825000	-0.96408200
H	2.65988700	-1.94242000	-2.17816000
C	1.15767600	-2.40024800	0.10213800
H	0.91094900	-3.06871100	-0.71161900
C	0.84599800	-2.69891700	1.42302400
H	1.42131400	-2.17644100	2.18289000
C	-0.32608800	-3.31410400	1.86572100
H	-0.59304900	-3.17264500	2.90707900
C	-1.33232700	-3.80067800	1.03788700
H	-2.27224700	-4.01084600	1.53599800
C	-0.75407700	-1.19805800	-0.44755800
C	-1.79432200	-1.64371100	0.37450300
H	-1.86168000	-1.26948000	1.38868000
C	-3.07040300	-2.10645300	-0.15338900
C	-0.88527800	-1.48046100	-1.89617500
C	-2.11886100	-2.14662600	-2.43070500
C	-3.15313000	-2.39533400	-1.61111700
O	-4.06722000	-2.26804400	0.56040100
O	-0.02433900	-1.15210000	-2.71193600
C	-1.64206800	2.05590000	1.66295500
H	-1.33284400	2.97618400	2.16713300
H	-2.71766400	1.94877100	1.83312400
H	-1.14426100	1.21849700	2.14695800
C	-1.99750900	3.34660900	-0.48004200
H	-1.79163200	3.36771300	-1.55034100
H	-3.08219400	3.33784600	-0.33542900
H	-1.62724100	4.27679200	-0.03862700
C	-1.11065600	-4.54461900	-0.25127000
H	-0.32790300	-5.29366400	-0.10481500
H	-2.03394700	-5.04610800	-0.53649500
H	-0.78355600	-3.92278400	-1.08343100
C	-2.12462300	-2.48564900	-3.88798900
H	-1.37221900	-3.25316000	-4.08407900
H	-3.10050500	-2.85903000	-4.18748700
H	-1.85882300	-1.60851000	-4.47856900

O	-4.28992200	-3.00372300	-2.06056100
C	-5.43607800	-2.14023900	-2.12935400
H	-6.25788700	-2.76179500	-2.47474500
H	-5.66176200	-1.72854800	-1.14830600
H	-5.24855900	-1.33996400	-2.84774100
H	1.73488600	-4.03922700	-3.40349200
O	0.85383400	-3.79174400	-3.10300100
H	0.76624800	-2.84476400	-3.28947700
H	-3.73283800	-2.73063000	3.87736100
O	-3.12817900	-2.29544800	3.26747300
H	-3.61286600	-2.23095400	2.42727400
O	-4.46651500	-5.08285100	-0.03312800
H	-4.49729400	-4.83872600	-0.96718200
H	-4.62260500	-4.23107700	0.39713500