Supporting Information

Cartesian coordinates and energies of all optimized compounds

N-phenyliminopropadienone 4a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -476.0097355 (hartree), -1249166.03933856 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.1990392611, 1.1169429912, 0.0010537769; C, 0.933004339, -0.260587886, -0.001278791; C, 1.9885614669, -1.1795942484, -0.0035953091; C, 3.301694662, -0.7211468685, -0.0035732243; C, 3.5714452416, 0.6469884678, -0.0012581475; C, 2.5165243955, 1.5604602965, 0.0010463376; N, -0.369958068, -0.7373048995, -0.0013414462; C, -1.535943019, -0.4565870186, -0.000101481; C, -2.8038213884, -0.2627313626, 0.0010116758; C, -4.0557481976, -0.0566829928, 0.0029095016; O, -5.2088927052, 0.1333431048, 0.0048016952; H, 1.7645565444, -2.2390902052, -0.0053776956; H, 4.1164612344, -1.4358889262, -0.0053718496; H, 4.595875387, 1.0001594469, -0.0012476553; H, 2.719587083, 2.6253266365, 0.00284946; H, 0.3758273013, 1.8215142345, 0.0028382682.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -476.0156165 (hartree), -1249181.47252181 (kJ mol^{-1}).

N-(2,6-difluorophenyl)-iminopropadienone 4b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -674.53803 (hartree), -1770152.86973754 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.7870390524, -0.0004785935, -2.7188612944; C, -0.7378521097, -0.0002861999, -1.3376568143; C, 0.4699015886, -0.0000157592, -0.6218030347; C, 1.6468827436, 0.000051903, -1.3842346999; C, 1.6347139355, -0.0001354297, -2.7676794828; C, 0.4103538626, -0.0004015053, -3.4332654409; N, 0.5262057831, 0.0001763895, 0.7482692333; C, -0.1435205577, 0.0002136441, 1.7498017054; C, -0.7382211728,

0.000278449, 2.8804880709; C, -1.3745215501, 0.0003362465, 3.9803165348; O, -1.9545098326, 0.0003896857, 4.9923679763; H, 2.5757988497, -0.0000712063, -3.3020106809; H, 0.3883805203, -0.0005499048, -4.5157500707; H, -1.7499096998, -0.0006839624, -3.2130686681; F, -1.8823141742, -0.0003561363, -0.6268456034; F, 2.8216677723, 0.000309062, -0.7318913175.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -674.5442462 (hartree), -1770169.18256763 (kJ mol^{-1}).

N-(2-pyridyl)-iminopropadienone 4c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -492.0510402 (hartree), -1291262.34864382 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.6890969648, -0.0002348077, -2.8660088727; C, -0.6834419176, -0.0001056555, -1.47887201; C, 0.5595501216, -0.0001044388, -0.8255115014; N, 1.7286538281, -0.000220369, -1.4653445865; C, 1.7000855586, -0.0003434682, -2.7997812574; C, 0.5260468336, -0.0003568932, -3.5490489176; N, 0.6209589916, 0.000021981, 0.5602025052; C, -0.0161240781, 0.0001480242, 1.5767428701; C, -0.607108576, 0.000283023, 2.7132100112; C, -1.2004184933, 0.0004167228, 3.8356612012; O, -1.7482523594, 0.0005396826, 4.8665473768; H, 2.6683287475, -0.0004359319, -3.2915027821; H, 0.5654873684, -0.0004597448, -4.6311759951; H, -1.629358354, -0.0002400222, -3.4055483085; H, -1.6026835282, -0.0000080817, -0.9065065006.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -492.0591184 (hartree), -1291283.54781759 (kJ mol^{-1}).

N-(3-pyridyl)-iminopropadienone 4d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -492.0475109 (hartree), -1291253.0868969 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.663464287, -0.0002321635, -2.8905581836; C, -0.6949216102, -0.0001340935, -1.5027922852; C, 0.5242167521, -0.0001436762, -0.8143205484; C, 1.7131419714, -0.0002520512, -1.5582609424; N, 1.7398857841, -0.0003458273, -2.8881574177; C, 0.5716994887, -0.0003357944, -3.5386224029; N, 0.5961275879, -0.0000546045, 0.5671986008; C, -0.0372331577, 0.0000597413, 1.5883554849; C, -0.6170367391, 0.0001350063, 2.7299103275; C, -1.205308024, 0.0004952737, 3.8555295517; O, -1.7471316893, 0.0007756893, 4.8892785786; H, 2.6663448857, -0.0002616025, -1.0384370758; H, 0.6259992129, -0.0004135548, -4.6227693784; H, -1.5825356136, -0.0002287808, -3.4644921985; H, -1.6314149398, -0.0000520089, -0.957264268.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -492.0551753 (hartree), -1291273.2001582 (kJ mol^{-1}).

N-(4-pyridyl)-iminopropadienone 4e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -492.0487204 (hartree), -1291256.26092089 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.6136445992, -0.0002575709, -2.8780550754; C, -0.6520893737, -0.0001158765, -1.4882450956; C, 0.56485864, -0.0001077255, -0.7942045389; C, 1.7523436791, -0.0002418639, -1.530646505; C, 1.6662969742, -0.0003771996, -2.9190801964; N, 0.5141152178, -0.0003870443, -3.597017257; N, 0.6186937265, 0.0000285589, 0.5883895372; C, -0.0425746629, 0.0001621953, 1.5932266526; C, -0.646877267,

0.000305263, 2.72031385; C, -1.2648307496, 0.0004476202, 3.8307875035; O, -1.8320378352, 0.0005781302, 4.8496342591; H, 2.7097773263, -0.0002395463, -1.0257043936; H, 2.5732667195, -0.0004832012, -3.5163893533; H, -1.5415968747, -0.0002673542, -3.4426250627; H, -1.5957029449, -0.0000145938, -0.9565407938.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -492.0562851 (hartree), -1291276.112545 (kJ mol^{-1}).

Complex a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.863827 (hartree), -2668499.53811552 (kJ mol-1). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.9688081208, 5.2584310915, -0.3463384364; C, 1.7425254508, 4.1263020001, -0.085973091; C, 1.1951856822, 2.8503499564, -0.1775160775; C, -0.1536982444, 2.7141806487, -0.5390372914; C, -0.93657059, 3.8445997951, -0.7970332144; C, -0.3716069741, 5.1123585118, -0.7013513583; N, -0.7493395666, 1.4545523506, -0.6452930087; C, -0.4459749045, 0.2862978559, -0.628429421; C, -0.2430893544, -0.9755558228, -0.6378822317; C, 0.0041629295, -2.216454246, -0.5439047226; O, 0.2844897419, -3.3502545194, -0.4809742666; N, 3.6552233983, -2.6370648087, -0.497702556; C, 3.9391174512, -2.3981258972, -1.9121572824; C, 4.6905851689, -3.429655776, 0.1636443282; N, 3.302075473, 0.2473676113, 1.0164352437; C, 4.6264912185, 0.8464124607, 1.1298325779; C, 2.6854038973, 0.000463126, 2.3149727333; N, -3.1999101941, -2.7600367045, 0.0875631667; C, -3.4755036153, -3.5307205299, 1.290826228; C, -3.7654614894, -3.3578286718, -1.1127555683; N, -4.1115127929, 0.3927547796, 0.3854993344; C, -4.2849718084, 0.7660471472, 1.7874170198; C, -5.2416276039, 0.7834758744, -0.4533690653; H, -1.9754469131, 3.7162407734, -1.0760196549; H, -0.9797523243, 5.9862119644, -0.905459799; H, 1.4075661631, 6.2467542952, -0.2719588998; H, 2.7849027299,

4.2349602395, 0.1922489613; H, 1.7992450627, 1.9706516943, 0.0356236688; H, -3.5371909964, -1.8035651716, 0.195635243; H, -4.8530501303, -3.5469680588, -1.048624302; H, -3.2773818126, -4.3169594842, -1.3168292328; H, -3.584614759, -2.7054384607, -1.9708727853; H, -2.9669327073, -4.4993562408, 1.2373841922; H, -4.5503697434, -3.7297273319, 1.4582910427; H, -3.0879576647, -3.0019576169, 2.1653342588; H, -3.2599065649, 0.8138997041, 0.0271348132; H, -5.4862929279, 1.8575549572, -0.3930041277; H, -6.1318153409, 0.2235341368, -0.1512905474; H, -5.0301678519, 0.5363505303, -1.4960966093; H, -5.1200509667, 0.2027769448, 2.2148288271; H, -4.4932508444, 1.8389110327, 1.9359186687; H, -3.3851116005, 0.5094653954, 2.3506195374; H, 3.3726404656, -0.6344072764, 0.5052622029; H, 3.3118746699, -0.6033593107, 2.9952911158; H, 2.4774703541, 0.9515159231, 2.8173057605; H, 1.7338340114, -0.5184817102, 2.1777924389; H, 5.3252725117, 0.264142647, 1.756777022; H, 5.0695625121, 0.9554594974, 0.1367568695; H, 4.5486956973, 1.8458786203, 1.5718701483; H, 2.7638109391, -3.1159866923, -0.413963413; H, 4.1045626367, -3.3225362767, -2.4895999517; H, 3.1106544886, -1.8504745931, -2.3662464247; H, 4.8386549894, -1.7820232424, -2.0052054505; H, 4.8941719775, -4.3913241823, -0.3357525621; H, 5.626181045, -2.8627501905, 0.1880408871; H, 4.3958687257, -3.6334341032, 1.1954162135.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8682008 (hartree), -2668511.01603711 (kJ mol-1).

Complex b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.390973 (hartree), -3189483.35456943 (kJ mol-1). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -5.6673927244, -0.9945624975, -1.8261388999; C, -6.1898919775, -0.8630766707, -0.5406889895; C, -5.3502523843, -0.6154653433, 0.5443158352; C, -3.9903911977, -0.5019730953, 0.3231261613; C, -3.4152583106, -

0.6253152874, -0.9515985352; C, -4.3017253777, -0.8750721405, -2.0082136488; N, -2.0648319843, -0.5160455949, -1.1921749275; C, -1.037689549, -0.299658673, -0.5814000747; C, 0.1040530006, -0.0835641371, -0.0658158061; C, 1.2845792732, 0.1137231032, 0.3671887961; O, 2.3425315506, 0.306400517, 0.8160852106; N, 2.461892669, -0.5873416161, -2.4876265699; C, 3.3389567371, 0.4617565138, -2.9880008043; C, 3.1290983029, -1.8767379784, -2.3740831313; N, -0.2503860688, -0.814226137, -4.3279638568; C, -0.4069518135, 0.3867113996, -5.1463483645; C, -0.3167227297, -2.045807375, -5.1121195112; N, 4.2636794509, 1.6110502029, 3.2869645788; C, 5.4996936716, 0.8422332465, 3.4057399841; C, 4.4960440465, 3.0283512654, 3.0188246469; N, 2.1566243854, 1.68058038, 5.7536857242; C, 1.3657165284, 0.4620149645, 5.8221654044; C, 2.799289979, 2.0133115071, 7.0150433349; F, -3.7851572863, -1.0014378334, -3.2470520063; H, -6.2990963708, -1.1873832196, -2.6834157356; H, -7.2571753382, -0.9540965414, -0.3831609926; H, -5.7313283482, -0.5095515503, 1.5517945358; F, -3.1624747487, -0.2635891696, 1.3585639293; H, 1.6384428016, -0.670892682, -3.0851182531; H, 3.8214782695, 0.2174211236, -3.951977782; H, 4.1359443385, 0.6583593214, -2.2628613166; H, 2.7725047183, 1.3874399236, -3.1168187725; H, 3.9135832952, -1.8243929087, -1.6114538362; H, 3.6023088838, -2.2181159721, -3.3127521664; H, 2.4111149851, -2.6384706508, -2.0596172796; H, -0.9763656718, -0.829613113, -3.6180108989; H, -1.3281880119, 0.3886043525, -5.7521501237; H, 0.4424212389, 0.4769468748, -5.8303122792; H, -0.4153908706, 1.2709379301, -4.5051453538; H, 0.5378636636, -2.0917297279, -5.7940001835; H, -1.2346146949, -2.1329181823, -5.7167760415; H, -0.2598804004, -2.9102599329, -4.4468381841; H, 2.8536205269, 1.6042508041, 5.0123308234; H, 1.9294806694, -0.4192490174, 6.1823933888; H, 0.5158778638, 0.6049208323, 6.4989412745; H, 0.9642113174, 0.2264600764, 4.8333825933; H, 3.4302576487, 1.202262193, 7.4253554229; H, 3.4263019297, 2.8995640803, 6.8881753633; H, 2.0414015749, 2.2502547598, 7.7701369002; H, 3.6933422206, 1.2183361756, 2.5449209726; H, 5.1104171267, 3.2119146395, 2.1212286127; H, 3.5392578179, 3.5400003349, 2.895627563; H, 5.0092584391, 3.4825910643, 3.8719841038; H, 6.1650001563, 0.9390489326, 2.5310618413; H, 6.0566909542, 1.1775463713, 4.2860879372; H, 5.2639131599, -0.2154808571, 3.5425258478.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.3983146 (hartree), -3189502.62072453 (kJ mol-1).

Complex c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.908018 (hartree), -2710603.42177834 (kJ mol-1). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.4774786201, 2.4800742794, -0.2805106723; N, -1.4840923394, 3.3462070065, -0.4076636971; C, -1.1737148728, 4.6435531966, -0.4692483664; C, 0.1300762284, 5.1278675337, -0.4086072031; C, 1.1679601671, 4.2062471736, -0.2727245356; C, 0.8745038191, 2.8511335389, -0.2045317722; N, -0.848469347, 1.1386879512, -0.2216243686; C, -0.3719644854, 0.0337381348, -0.150606108; C, 0.029515501, -1.1764072795, -0.0825793867; C, 0.3917783957, -2.3898063424, -0.0153400328; O, 0.7728840941, -3.4935046734, 0.0426545579; N, -4.1648093169, 0.2297081318, 0.0873272983; C, -5.1114400153, 0.4688245603, -0.9995599078; C, -4.7081128472, 0.5836456511, 1.3965438867; N, -3.1326401549, -2.9155833966, 0.104781746; C, -3.6327744458, -3.611187419, -1.0714950404; C, -3.5429564891, -3.5421597183, 1.3524252715; N, 3.5001280833, 0.7254022661, 0.6999118264; C, 3.1875644851, 0.5798072271, 2.1179060806; C, 4.736959785, 1.4643574273, 0.4722462513; N, 4.0318210001, -2.2901482826, -0.4950262053; C, 5.2358980296, -2.7940577714, 0.1641018491; C, 4.1597852038, -2.2389755025, -1.9509511003; H, 0.3223602993, 6.1922782829, -0.4643633379; H, -2.012494266, 5.3256463564, -0.5731338636; H, 2.1988306488, 4.5382182507, -0.2190900955; H, 1.6553237556, 2.1020468831, -0.0876443058; H, -3.4337873316, -1.9405861698, 0.0885491335; H, -4.7311269545, -3.7399220677, -1.0825416622; H, -3.1855710893, -4.6093348681, -1.1328944982; H, -3.3463473862, -3.0643846038, -1.973418213; H, -3.0894984697, -4.5356954251, 1.4379401338; H, -4.6372040327, -3.6687603065, 1.4518766453; H, -3.1925444595, -2.9449738035, 2.1980462276; H, -3.3211492905,

0.7710805516, -0.0794853093; H, -5.4938860253, 1.5027346126, -1.0297182196; H, -5.9697224356, -0.2019273594, -0.8928789574; H, -4.6342842286, 0.2521956051, -1.9579536282; H, -5.5429380008, -0.0810666495, 1.639899758; H, -5.0766473388, 1.6215040872, 1.4534481746; H, -3.9402348971, 0.4503027748, 2.1619566648; H, 3.5804380591, -0.2017596531, 0.2783711525; H, 4.0073595084, 0.133885831, 2.7079073512; H, 2.9638820465, 1.5593043123, 2.5544124374; H, 2.3015872422, -0.0481233777, 2.2367555298; H, 5.6111022707, 1.0384490877, 0.9958293617; H, 4.960238816, 1.4920758565, -0.5972046689; H, 4.6243939078, 2.4983454454, 0.816648853; H, 3.245192915, -2.8837044704, -0.250746707; H, 4.4394871249, -3.205143016, -2.4018334978; H, 3.2159836349, -1.9122945147, -2.3924322837; H, 4.9280230526, -1.5091774512, -2.2240008829; H, 5.5615839314, -3.77946738, -0.2078091757; H, 6.0596212306, -2.0908460222, 0.0084551863; H, 5.0617904994, -2.8727072843, 1.2394547537.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9128882 (hartree), -2710616.20237502 (kJ mol-1).

Complex d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9032816 (hartree), -2710590.9923056 (kJ mol-1). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, -5.1159858787, 0.0352818725, 0.0815232385; C, -5.0966211832, 0.1404270294, 1.4145408321; C, -3.9189068333, 0.2224642082, 2.1572390868; C, -2.6945224947, 0.1962233465, 1.5004761151; C, -2.7120190944, 0.0881779742, 0.1041168236; C, -3.9464522156, 0.0096933508, -0.5534693807; N, -1.5465879626, 0.0504114352, -0.6600879264; C, -0.3523834048, 0.1518349715, -0.4905422243; C, 0.9178436243, 0.2469828693, -0.4306765471; C, 2.1842430762, 0.3076667995, -0.350274804; O, 3.3414014727, 0.3910738418, -0.2140636164; N, 2.4255098959, -0.7753014482, -3.3526487107; C, 3.0424834018,

0.1932891264, -4.2474750161; C, 3.12384682, -2.052501332, -3.3301394972; N, -0.7777325817, -1.1848757865, -4.0167656601; C, -1.2469934035, -0.3327178125, -5.1071724105; C, -1.1346980235, -2.5903455542, -4.1974954997; N, 2.8989675152, 1.6391573219, 3.0020351147; C, 3.7758498489, 1.4309811482, 4.1536356479; C, 2.6171171976, 3.0522317731, 2.750864533; N, 0.0914972128, 0.0540422781, 3.5941656208; C, 0.3822348929, -1.3761505428, 3.6055339615; C, -0.3772257742, 0.5394711261, 4.8877183528; H, -3.9705252105, -0.0746145146, -1.6361681309; H, -6.0637188077, 0.1586833967, 1.9080040154; H, -3.960790012, 0.3053486089, 3.2371165988; H, -1.7548867408, 0.2508384292, 2.0494881117; H, 1.4470675036, -0.914664305, -3.6060299586; H, 3.1614238785, -0.169615381, -5.2849196816; H, 4.0380621093, 0.4605129742, -3.8772715896; H, 2.4427491397, 1.1066092471, -4.2743577167; H, 4.1243807043, -1.9221610049, -2.9041174345; H, 3.2458295417, -2.5124676175, -4.3278955358; H, 2.5828081671, -2.758557256, -2.6950217323; H, -1.1589385341, -0.8496345958, -3.1373482604; H, -2.330544935, -0.4141921387, -5.2957841024; H, -0.7277799256, -0.6028732502, -6.0316464398; H, -1.0136857697, 0.7111016213, -4.8858921811; H, -0.6117233978, -2.9907577865, -5.0711976407; H, -2.2145339823, -2.7553596882, -4.3486324115; H, -0.8172633192, -3.166230047, -3.3254200776; H, 0.9367365358, 0.5645448459, 3.3310961994; H, 1.0902535371, -1.6770922724, 4.3974174377; H, -0.541587732, -1.9446375956, 3.7578878127; H, 0.8021156025, -1.6745969175, 2.6420791089; H, 0.312438971, 0.3171222438, 5.7209770076; H, -0.5241892821, 1.6215612937, 4.8459882805; H, -1.3415130784, 0.0809348125, 5.1328774722; H, 3.3303806368, 1.2350109578, 2.1765227061; H, 3.5244002727, 3.6661987121, 2.6293514236; H, 2.0092896084, 3.1517851064, 1.8491406541; H, 2.0452405275, 3.4647493343, 3.5875766303; H, 4.7251487177, 1.987835675, 4.0898184177; H, 3.2631803783, 1.7504864629, 5.0658927925; H, 4.0065070999, 0.3681593124, 4.2541455786.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9090108 (hartree), -2710606.0271285 (kJ mol-1).

Complex e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9040106 (hartree), -2710592.90538001 (kJ mol-1). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.0883991409, 5.1105140721, -0.6818878447; N, 1.1997917791, 5.2115517286, -0.3400161293; C, 1.8508875267, 4.0689831567, -0.0898856424; C, 1.2790946036, 2.8025033335, -0.1637295373; C, -0.0713311154, 2.7217114731, -0.5271258854; C, -0.7703349145, 3.9028293928, -0.7885602647; N, -0.7390863283, 1.5028489519, -0.62787324; C, -0.4686501038, 0.3222843738, -0.6024372633; C, -0.3086225519, -0.9416001548, -0.6030763294; C, -0.1102950407, -2.193953693, -0.5099196096; O, 0.1354465595, -3.3331456539, -0.4485087353; N, -3.1988369486, -2.6536590621, 0.0748278642; C, -3.7805199079, -3.2747519438, -1.1065630267; C, -3.4424524396, -3.4120409008, 1.2934868528; N, -4.1470635819, 0.485082588, 0.3605513224; C, -5.2832721423, 0.8502663274, -0.4825463193; C, -4.3347235998, 0.8552913095, 1.7619554177; N, 3.5514696652, -2.7184469633, -0.5085161295; C, 4.5836973489, -3.5131416723, 0.1560283394; C, 3.8353565631, -2.4885409033, -1.9247394081; N, 3.2791699966, 0.1714719614, 1.0106600609; C, 2.6918939993, -0.0691011379, 2.3244201214; C, 4.6167207584, 0.7479544757, 1.092613243; H, -1.8147254612, 3.872117424, -1.0727907732; H, -0.6063054584, 6.0441110988, -0.8824077894; H, 2.8964065702, 4.1683902965, 0.1878325188; H, 1.8625670127, 1.9117615589, 0.0629994444; H, -3.5474459709, -1.700283053, 0.1772052942; H, -4.8638103876, -3.4754859513, -1.0176785387; H, -3.2850773127, -4.2308001232, -1.3070165333; H, -3.6248473929, -2.6318601997, -1.9766870836; H, -2.9229836698, -4.3749308547, 1.2429755388; H, -4.5112611594, -3.6214658343, 1.4825082266; H, -3.0461692816, -2.8668017619, 2.1538178821; H, -3.3048717207, 0.9273907146, 0.0054692914; H, -5.552364235, 1.9182432918, -0.4223853246; H, -6.1612541049, 0.2698917539, -0.183640171; H, -5.0625354691, 0.608573316, -1.5246065971; H, -5.1582087081, 0.2731333946, 2.186293281; H, -4.5685390464, 1.9229417716, 1.9085538718; H, -3.4315888866, 0.6200854498, 2.3292930391; H, 3.3224394305, -0.710433764, 0.4966511272; H, 3.3253805762, -

0.6854410314, 2.986296156; H, 2.5133679134, 0.8835723546, 2.8347731417; H, 1.7283660217, -0.5716226764, 2.2107878833; H, 5.3200830637, 0.1514179016, 1.7000727682; H, 5.0366040133, 0.8529851711, 0.0891512514; H, 4.5668739693, 1.7468476678, 1.5394955689; H, 2.6578922469, -3.1924804457, -0.4211076437; H, 3.9954406645, -3.4167496201, -2.497333315; H, 3.0097224873, -1.9385938335, -2.3813119265; H, 4.7380069786, -1.87782044, -2.0215772285; H, 4.7822558242, -4.4778561816, -0.3391363341; H, 5.5217174663, -2.9503390678, 0.176957189; H, 4.2888804175, -3.7105225802, 1.1889823659.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9100914 (hartree), -2710608.86288736 (kJ mol-1).

5a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.2559309 (hartree), -1604085.15473431 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.8010752926, 0.5660249439, 0.0130518365; N, -0.7196774037, 0.624305298, 1.2165614996; C, 0.4246063342, 0.6700196427, 2.0483105181; C, -1.00467572, 0.5098058533, -1.2929881418; C, -0.9426718907, -0.8075180664, -1.9728302455; O, -0.5319336559, -1.805807047, -1.3847052342; C, 1.6392040843, 0.0974856895, 1.6546678561; C, 2.7289331153, 0.1467382404, 2.517901167; C, 2.6154877366, 0.763928661, 3.7644533369; C, 1.3994719061, 1.3239004421, 4.1535118544; C, 0.2983858219, 1.2679125889, 3.3033161258; N, -1.3526258343, -0.8501694493, -3.2860564002; C, -1.8889605272, 0.2841977249, -4.0240126511; C, -1.1562544382, -2.078911193, -4.0447977785; H, -1.1493033392, 1.4432551355, -1.8199143949; H, 1.7102161739, -0.3961911422, 0.6923790863; H, 3.6686110127, -0.3029591159, 2.2177912088; H, 3.4685386634, 0.7990844623, 4.4322039637; H, 1.3037817821,

1.7966015764, 5.1242683468; H, -0.658042568, 1.6849007844, 3.594345886; H, -1.1040219282, 0.8732217268, -4.5165493398; H, -2.4709694463, 0.9379244462, -3.3757054786; H, -2.5636933683, -0.0890429178, -4.7976593497; H, -0.7224451849, -2.8281401851, -3.3877369971; H, -0.4832124183, -1.9046670928, -4.8924881625; H, -2.1125742434, -2.4479894064, -4.4303318585.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.266077 (hartree), -1604111.78058376 (kJ mol^{-1}).

5b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7828437 (hartree), -2125068.35921436 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.6685329968, 0.5476392033, -3.0165379659; C, 0.639411297, -0.071076362, -1.7597394922; C, 1.8565749046, -0.5863433722, -1.2925443998; C, 3.0341286481, -0.4975366259, -2.0125078516; C, 3.0130131128, 0.1362934774, -3.2536051928; C, 1.8292594444, 0.6635216984, -3.7633628424; N, -0.5732030597, -0.1612403776, -1.0783201492; C, -0.8470977815, -0.4582595568, 0.0632249498; C, -1.2947280892, -0.7535994163, 1.2693107731; C, -1.3959575112, 0.3264525165, 2.2828075101; N, -1.9642346319, -0.0106651738, 3.4910206529; C, -1.9515845552, 0.9718742152, 4.5679849806; O, -0.9904180167, 1.4608000612, 2.0448108548; C, -2.4420662461, -1.3432000352, 3.8334038602; H, -1.5131619504, -1.7912697336, 1.4811175449; F, 1.8616843299, -1.2026721572, -0.0957946469; H, 3.9414952673, -0.9161426606, -1.5968993034; H, 3.9275507866, 0.2190927287, -3.82773647; H, 1.7904535301, 1.1593511413, -4.7244033772; F, -0.4746419628, 1.0500841551, -3.5069885696; H, -1.6327692066, -2.0102773225, 4.1578900897; H, -2.9698034151, -1.8038136062, 2.9981260069; H, -3.1544793167, -1.2554411428, 4.6556504098; H, -1.5664928345, 1.9101205046, 4.1773125075; H, -1.3129631139, 0.6360019217, 5.3937637839; H, -2.964720398, 1.1280141045, 4.9522314181.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7947991 (hartree), -2125099.73310979 (kJ mol^{-1}).

5c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2982425 (hartree), -1646184.10639159 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, 0.6505964632, -0.2042225601, -3.3766176164; C, 0.654691779, 0.1362767338, -2.0935556956; C, 1.8058992108, 0.4662602275, -1.3672424183; C, 3.0213106365, 0.4209052576, -2.0368315364; C, 3.042583878, 0.0483446544, -3.3802863311; C, 1.8333514476, -0.257600829, -3.9979312731; N, -0.6131145302, 0.2240543437, -1.4665846504; C, -0.9630957856, -0.2170125578, -0.4007081886; C, -1.4259637798, -0.6391036457, 0.76347758; C, -1.0659483749, 0.1360505828, 1.9772747075; N, -1.7266117277, -0.1832249456, 3.1387543116; C, -1.2918928884, 0.4277376535, 4.3886159697; O, -0.2016508044, 1.0110812425, 1.9345381871; C, -2.8059264028, -1.1555303096, 3.2374125889; H, -1.9816663581, -1.5659944863, 0.7869324802; H, 1.7263477073, 0.7530904193, -0.3255059585; H, 3.9385203865, 0.671047198, -1.5157705748; H, 3.9696576333, 0.0011811179, -3.9382460606; H, 1.8048977644, -0.5516903128, -5.0429474864; H, -2.438979474, -2.1651134901, 3.463578238; H, -3.3937511246, -1.1860322629, 2.3212630769; H, -3.4774711259, -0.8531725431, 4.0442219412; H, -0.4481773781, 1.0810848187, 4.1825526575; H, -0.9900530654, -0.3439266921, 5.1058758911; H, -2.1022682892, 1.016661822, 4.8315235673.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.3096969 (hartree), -1646214.16554041 (kJ mol^{-1}).

5d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2946848 (hartree), -1646174.77011612 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.7199024717, 0.0383620319, -3.4708073209; C, 0.6732033167, 0.0955102912, -2.0751195867; C, 1.8713754283, 0.1656467854, -1.3610506494; C, 3.0597578985, 0.1513312574, -2.0803367376; C, 3.004499324, 0.0676746405, -3.4715226808; N, 1.8600148466, 0.0118652178, -4.1600574207; N, -0.5891056589, 0.1331463583, -1.4435102656; C, -0.9015579631, -0.2783593814, -0.3502164289; C, -1.3393399805, -0.6858806435, 0.8277192453; C, -1.0899434005, 0.1759629887, 2.0127130298; N, -1.7513439596, -0.1514875124, 3.1715553406; C, -1.417652152, 0.5610837754, 4.3988915424; O, -0.3119507003, 1.1257398186, 1.9474457509; C, -2.7322832438, -1.2202659925, 3.2951751816; H, -1.7999944868, -1.6626902235, 0.8882185405; H, 1.8564879459, 0.2508456229, -0.2802582381; H, 4.0156039296, 0.210358974, -1.5733557533; H, 3.9176372859, 0.0550033321, -4.0590003537; H, -0.2067636253, 0.0053221692, -4.0358900187; H, -2.2761086257, -2.1716590915, 3.5981873377; H, -3.2766372778, -1.3660138913, 2.3635273504; H, -3.4629558171, -0.9397935392, 4.0573958057; H, -0.6422012739, 1.290288492, 4.1795831143; H, -1.0563248492, -0.1389038482, 5.1607362449; H, -2.2978643949, 1.0802604894, 4.7927028153.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.3061273 (hartree), -1646204.79803643 (kJ mol^{-1}).

5e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2954827 (hartree), -1646176.86400099 (kJ mol^{-1}). Structure definition (3D

Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.6866108565, -0.0759464732, -3.4632649772; C, 0.6330259167, 0.1416502391, -2.0878184103; C, 1.8239123516, 0.3364600983, -1.3849421604; C, 3.016675406, 0.2826862115, -2.100320557; N, 3.091409742, 0.0522323737, -3.4155310332; C, 1.9388992819, -0.1232232203, -4.0694804268; N, -0.6220880237, 0.2220094603, -1.4461000867; C, -0.9497875623, -0.2150033812, -0.3677406592; C, -1.3985275807, -0.6421153717, 0.7980895819; C, -1.0672395289, 0.1513916796, 2.011485852; N, -1.7170107474, -0.1871765052, 3.1728013967; C, -1.3087946166, 0.4496461841, 4.4194413029; O, -0.2362356905, 1.0559253241, 1.96281825; C, -2.7545851425, -1.2034038464, 3.2788350572; H, -1.9253985514, -1.5860635451, 0.8260338465; H, 1.8089818252, 0.5413967213, -0.3210156023; H, 3.9616401964, 0.4319367213, -1.5860066734; H, 2.0167957215, -0.3040553982, -5.1376429263; H, -0.2224228349, -0.207743218, -4.0365037193; H, -2.3452873174, -2.1936317087, 3.516991067; H, -3.3386469715, -1.2688483064, 2.362160055; H, -3.440774515, -0.9212357967, 4.0805431416; H, -0.4918216885, 1.1351483543, 4.2103625581; H, -0.9772448528, -0.3045843405, 5.1418417591; H, -2.143248575, 1.0079679036, 4.8567909372.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.3068669 (hartree), -1646206.73892783 (kJ mol^{-1}).

6a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.2404959 (hartree), -1604044.64951692 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.3089938393, 0.1447917488, -0.1843170233; N, 0.3559943625, -0.7213244866, -0.3187874085; N, 1.2014666386, 1.5220378721, -0.1912294468; C, 2.6724282984, -0.394341678, -0.0562248721; C, 2.8286455719, -1.6884963272, 0.1815796846; O, 3.0136725583, -2.8069397223, 0.3977203453; C, -1.0029950312, -

0.4772478648, -0.1029126718; C, -1.9400938808, -1.0264660929, -0.9951650126; C, -3.3057507466, -0.8891081332, -0.7693936376; C, -3.7747449713, -0.2206906665, 0.3623779732; C, -2.8543940719, 0.3064639773, 1.2680289299; C, -1.4860414684, 0.1837655979, 1.0421766459; C, 0.1184242522, 2.2036202265, -0.8897525248; C, 2.2353617827, 2.3944206281, 0.3481274226; H, 3.572602651, 0.1799547042, -0.2279382572; H, -1.5723180253, -1.5642978949, -1.8615421811; H, -4.009104548, -1.3163389348, -1.4763171446; H, -4.8391725533, -0.123363082, 0.5419024046; H, -3.2035454548, 0.8119594752, 2.1624754197; H, -0.7795156414, 0.5808270284, 1.7628693033; H, -0.3957277908, 1.514502519, -1.5550284501; H, 0.5423362517, 3.0150517266, -1.4909571961; H, -0.6187933456, 2.625869199, -0.1981401716; H, 2.9067444205, 2.7792574568, -0.432395373; H, 2.8247711824, 1.8748111873, 1.1017118666; H, 1.7611139343, 3.2520221976, 0.8345655195.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.2485502 (hartree), -1604065.78597124 (kJ mol^{-1}).

6b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7748648 (hartree), -2125047.42062809 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.9300290912, -0.3312036978, -1.4139750457; C, 0.8877016392, -0.2649610442, -0.0106020092; C, 2.1515203306, -0.2111171243, 0.6036504409; C, 3.3466963403, -0.2075827511, -0.0935745759; C, 3.3206207758, -0.2728655147, -1.4860542897; C, 2.0997831356, -0.3373556973, -2.1541685084; N, -0.2627432567, -0.411309414, 0.7448176578; C, -1.3688907712, 0.2474066544, 0.5679465553; C, -2.578413194, -0.3494526327, 1.1464104484; C, -2.5400697789, -1.6135427655, 1.5443186179; O, -2.5587818129, -2.7119766421, 1.8947378219; N, -1.5243202289, 1.4673969604, -0.0420733223; C, -2.7906369672, 1.9133466951, -0.6100413111; C, -0.4169492992, 2.4034931196, -0.1839466488; H, -3.4867891697,

0.1998455337, 1.3522310592; F, 2.1897272502, -0.1400138574, 1.9539175723; H, 4.2768105917, -0.1562865403, 0.4583367334; H, 4.2468230753, -0.2757872014, -2.0468184673; H, 2.0404374557, -0.4003772416, -3.2335735688; F, -0.2549019355, -0.4151470094, -2.0770951865; H, 0.3554492845, 2.1873462918, 0.5508933244; H, -0.7920441812, 3.4145439425, 0.0015313852; H, 0.0289545405, 2.3771399743, -1.1845699019; H, -3.2633046701, 2.6905755922, 0.0042505478; H, -3.4768252231, 1.0770124544, -0.7240699019; H, -2.6115884472, 2.3286438582, -1.6065076465.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7838628 (hartree), -2125071.03358216 (kJ mol^{-1}).

6c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2847464 (hartree), -1646148.6893223 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.0632126407, -0.5557883843, -1.452219446; C, 1.0728485605, -0.3461508386, -0.0563663904; N, 2.2116990102, -0.1039347659, 0.6120501235; C, 3.3533076733, -0.0596539079, -0.0808327879; C, 3.4428400167, -0.2525701438, -1.4557499995; C, 2.2593970003, -0.5068040149, -2.1503658178; N, -0.0873622126, -0.501864951, 0.6915269522; C, -1.1792232278, 0.1724628017, 0.5424980672; C, -2.401071156, -0.3987878684, 1.1312316274; C, -2.3874304481, -1.6570650429, 1.5458238583; O, -2.4232049872, -2.7510330775, 1.9100181525; N, -1.3170462801, 1.3991897309, -0.073242999; C, -2.6010722523, 1.9145551026, -0.5280834373; C, -0.2003688757, 2.3345847721, -0.1697346018; H, -3.2968395314, 0.1699477366, 1.3391568718; H, 4.2488598662, 0.1406371713, 0.5024073395; H, 4.4008311959, -0.2105980395, -1.9592217962; H, 2.2718555974, -0.6717994199, -3.2227005842; H, 0.1278987524, -0.7698748204, -1.9558379778; H, 0.5895078261, 2.05228347, 0.5224608879; H, -0.5554569822, 3.3337986595, 0.1024114695; H, 0.2175879901, 2.3759757851, -1.181513806; H, -3.0498929561,

2.6116217293, 0.1931845627; H, -3.2982892623, 1.1009944958, -0.7207594181; H, -2.4560958107, 2.4528529011, -1.4692777391.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2961557 (hartree), -1646178.63011769 (kJ mol^{-1}).

6d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2810417 (hartree), -1646138.96728285 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.0679337214, -0.3252760016, -1.4735448432; C, 1.0600918735, -0.3339464441, -0.0694805297; C, 2.3165054867, -0.3558105443, 0.5683768769; N, 3.4840717414, -0.333469913, -0.070620669; C, 3.4669495061, -0.3116735649, -1.4086195137; C, 2.2851722832, -0.3152502788, -2.1458808522; N, -0.0900353176, -0.4583990779, 0.705756753; C, -1.1960825328, 0.1944396559, 0.528170373; C, -2.3975013057, -0.3665637893, 1.1620057228; C, -2.3493105232, -1.6012080238, 1.6428153761; O, -2.3572782385, -2.67373649, 2.0665813447; N, -1.3661659929, 1.3813818342, -0.155284873; C, -2.6701169084, 1.8427917422, -0.6139642352; C, -0.2854153837, 2.3528624146, -0.2823611632; H, -3.3063818514, 0.1901813435, 1.3443787848; H, 2.3473746135, -0.39472362, 1.6538208367; H, 4.4326682968, -0.3003507233, -1.9049654027; H, 2.3186614989, -0.3178298624, -3.2298725568; H, 0.1321937507, -0.346388669, -2.021529651; H, 0.5241230922, 2.1107527622, 0.4017622955; H, -0.6704586793, 3.3446726398, -0.0240419935; H, 0.12162435, 2.3889663237, -1.2987939233; H, -3.1416694402, 2.536217444, 0.0962039883; H, -3.3377668241, 1.0007802354, -0.7889171038; H, -2.5465932189, 2.3688331475, -1.5647577775.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version =

AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2923179 (hartree), -1646168.55879127 (kJ mol^{-1}).

6e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2845318 (hartree), -1646148.12615938 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.0816733495, -0.3278751332, -1.4323018213; C, 1.0628313996, -0.3249252773, -0.024420651; C, 2.3141054619, -0.3433056274, 0.6155120211; C, 3.4732021991, -0.3333075884, -0.1491940901; N, 3.4945430339, -0.3237687268, -1.4887735279; C, 2.3026860794, -0.329630113, -2.096684136; N, -0.0951581027, -0.4318248588, 0.7305552985; C, -1.2082062203, 0.2015995768, 0.5185002912; C, -2.4175339068, -0.3809936166, 1.1147023203; C, -2.3583587264, -1.612872944, 1.6021647655; O, -2.3561539881, -2.6825234713, 2.0320679376; N, -1.3724225344, 1.3888645443, -0.1590079819; C, -2.671526972, 1.8503591843, -0.6336757127; C, -0.2848512444, 2.3524470245, -0.2933908999; H, -3.3441738906, 0.1553978618, 1.2648702012; H, 2.3611586297, -0.3701948772, 1.6976696818; H, 4.4431393162, -0.3386573339, 0.3414979668; H, 2.3229679137, -0.3388036932, -3.1838624287; H, 0.1557763645, -0.3516737661, -1.995625039; H, 0.5138753424, 2.1209149964, 0.4071324768; H, -0.6698532245, 3.3503987073, -0.0617588074; H, 0.1360631353, 2.3622142834, -1.3042937704; H, -3.1534592084, 2.537814925, 0.0747174817; H, -3.3348745351, 1.0085653262, -0.8247959039; H, -2.5342532337, 2.3823417148, -1.5787844031.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2958032 (hartree), -1646177.70507142 (kJ mol^{-1}).

TS21a

Optimised geometry: Program version = IA64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.1678541 (hartree), -1603854.01965617 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.0104753668, -0.0035073485, 0.004648356; N, 0.0014038149, -0.0138207526, 1.2166600914; C, 0.9921349526, -0.0100533392, 2.2042997309; C, -0.145264942, 0.1429777878, -1.2872182724; C, -0.2031209025, -0.7971735941, -2.3509559185; O, -0.1459406893, -1.9797234976, -2.5597998425; C, 2.3579808665, -0.0166503801, 1.8857044206; C, 3.3050386487, -0.0110219177, 2.9037357517; C, 2.9064694203, 0.000175633, 4.2412922077; C, 1.5480786686, 0.0052916963, 4.5557493; C, 0.5919268666, -0.0004825533, 3.5446569144; N, -0.4001583073, 0.2422842273, -3.5189733195; C, -1.7092327096, 0.0991894924, -4.1732294624; C, 0.7295715496, 0.2458682042, -4.4596018443; H, 2.6634533893, -0.0289941605, 0.8456787884; H, 4.3596865185, -0.0171485618, 2.6516499552; H, 3.6492165385, 0.0030489828, 5.0305624372; H, 1.230249092, 0.012746282, 5.5922222482; H, -0.4667377003, 0.0021019502, 3.7736785863; H, -2.4936605754, 0.1805111121, -3.4186799805; H, -1.7865055644, -0.875306454, -4.6654566848; H, -1.8389300474, 0.8921524335, -4.9123811014; H, 1.651192296, 0.4372903692, -3.9069493509; H, 0.5868818645, 1.0332729445, -5.2022243954; H, 0.8100449113, -0.7221305663, -4.9640405953; H, -0.3220651632, 0.9763612021, -2.4489772504.

TS21b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.696967 (hartree), -2124842.99773704 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.3553684224, 1.6814743017, 0.1792994776; C, -2.1094264891, 1.0889453812, 0.0853539796; C, -1.9305304315, -0.2926034799, -0.0895187469; C, -3.1045353587, -1.0570173638, -0.1666779019; C, -4.3687078537, -0.5001531807, -0.0793486903; C, -4.4904194009, 0.8767231228, 0.0954327445; F, -1.0045852854, 1.8584073799, 0.1655717404; N, -0.7014498175, -0.9110166437, -0.1747180442; C, 0.464776932, -

0.5656347854, -0.1744938179; C, 1.736851121, -0.335803381, -0.3247782731; C, 2.8103909635, -0.149362428, 0.5874006834; O, 3.0374343797, -0.1210706498, 1.766647141; F, -2.9851514929, -2.3862778485, -0.3341590923; N, 3.9391171817, 0.0767330004, -0.4835340986; C, 4.5029200364, 1.4336903138, -0.4200430915; C, 4.9568638025, -0.9846083571, -0.4555763435; H, -5.2340034712, -1.1466534837, -0.1474658809; H, -5.473447708, 1.3251625462, 0.1665191762; H, -3.4211474242, 2.7532623374, 0.315617206; H, 2.8551300459, -0.1105334059, -1.1907929777; H, 5.2159737155, 1.5718510448, -1.2349969363; H, 5.0071632228, 1.5941432888, 0.5380043707; H, 3.6942351277, 2.1594006242, -0.5231997526; H, 5.4908315173, -0.9777204288, 0.4997652018; H, 5.666609589, -0.8322594763, -1.2708844791; H, 4.4662504087, -1.9511689901, -0.5829920114.

TS21c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2095641 (hartree), -1645951.39256781 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.6445843246, 1.5112991189, -0.3042582766; C, -2.3778962689, 0.9619409041, -0.175882133; C, -2.2702483067, -0.4229832193, 0.0350072275; N, -3.3276671602, -1.2307192081, 0.1232953805; C, -4.5384952519, -0.6831128946, -0.0040635963; C, -4.7572256118, 0.6751051622, -0.2182439916; N, -1.0235182436, -1.0358959145, 0.1755716838; C, 0.1258671742, -0.6713371907, 0.0470440199; C, 1.3873768751, -0.4398523466, -0.191591533; C, 2.4382400224, 0.1206676346, 0.5827294012; O, 2.6395494168, 0.6310068511, 1.6522052363; N, 3.5861651451, -0.0778697576, -0.4737636714; C, 4.143751586, 1.198961237, -0.9436964199; C, 4.6083778177, -1.029430549, -0.0113947295; H, -5.3765675055, -1.3702289434, 0.0714355587; H, -5.7645118525, 1.0619430393, -0.3112446509; H, -3.7624134345, 2.5768174758, -0.467344887; H, -1.48605692, 1.574227402, -0.2315349139; H, 2.5199392291, -0.5500306961, -1.0628731244; H, 4.875943093, 1.0107790938, -1.7312160843; H, 4.624160979, 1.733562622, -0.1182538743; H, 3.3361051634, 1.8139512673, -1.3447954884; H, 5.1248989872, -

0.6379183071, 0.8705070046; H, 5.3318665564, -1.2046544699, -0.8097480905; H, 4.1243999124, -1.9726562702, 0.2478030964.

TS21d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2068678 (hartree), -1645944.31681675 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.5757898246, 1.059369772, -3.8004766933; C, -0.3666610119, 0.7055157734, -2.4740542381; C, 0.6398914431, -0.2224839133, -2.1837657178; C, 1.3823202335, -0.7493380637, -3.2494512079; N, 1.183336636, -0.409984834, -4.5215334486; C, 0.22042092, 0.4786052822, -4.7874121065; N, 0.937543306, -0.6512148634, -0.8902055477; C, 0.5326398289, -0.35741573, 0.2167678123; C, 0.2786464846, -0.0308793337, 1.4536926509; C, -0.7139488579, -0.458632829, 2.3794974037; O, -1.6762285922, -1.1743490603, 2.4495143579; N, -0.21840037, 0.3926105206, 3.6042458123; C, -1.2053655245, 1.3996270808, 4.0222052103; C, 0.2631361209, -0.4512979116, 4.7089342005; H, 2.1650623163, -1.4726109006, -3.0413414291; H, 0.0786690501, 0.735328575, -5.8328870179; H, -1.345718851, 1.7732556919, -4.069301499; H, -0.964939481, 1.1289904748, -1.6751396777; H, 0.6142214005, 0.6958803031, 2.6460287622; H, -0.7845610254, 2.0156319608, 4.8190493206; H, -2.1192412855, 0.9144570198, 4.3789091564; H, -1.4487833572, 2.0348876972, 3.1686289787; H, -0.5559347719, -1.0509425739, 5.1178445173; H, 0.6808570016, 0.1799389454, 5.4954268749; H, 1.0411018647, -1.118321236, 4.333495553.

TS21e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2084251 (hartree), -1645948.40355307 (kJ mol^{-1}). Structure definition (3D

Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.5395859167, 1.134479912, -3.758380922; C, -0.3319487061, 0.7402363948, -2.4416165424; C, 0.696580224, -0.1724629945, -2.1739911574; C, 1.4570660102, -0.6402931024, -3.2484343257; C, 1.1602097609, -0.1753034165, -4.5255570121; N, 0.1831947065, 0.696651501, -4.795915276; N, 0.986993762, -0.6317895251, -0.8896217355; C, 0.5486979767, -0.3749898022, 0.2157073422; C, 0.2600165114, -0.0867004961, 1.4519544236; C, -0.7285598445, -0.5556600539, 2.3626815431; O, -1.6600806664, -1.3115673195, 2.4142030312; N, -0.2850485433, 0.3087172213, 3.5952526975; C, -1.3164138906, 1.2759848482, 4.0009956308; C, 0.2124811718, -0.5195616366, 4.7049448744; H, 2.2581226728, -1.348674178, -3.0789935665; H, 1.7388731214, -0.5238076707, -5.3762593839; H, -1.3314731579, 1.8407257155, -3.992014962; H, -0.9526192103, 1.1262006308, -1.6417250788; H, 0.5527783094, 0.6459310035, 2.6449664038; H, -0.9290149943, 1.9088007922, 4.8014686887; H, -2.2139901966, 0.7550554882, 4.348366879; H, -1.5755286329, 1.9003614964, 3.1440801585; H, -0.5892539604, -1.150044285, 5.101531887; H, 0.5957884415, 0.1249871636, 5.498077532; H, 1.0197236788, -1.1564298967, 4.339044263.

TS12a

Optimised geometry: Program version = IA64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.2026177 (hartree), -1603945.24785023 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.0667993637, -0.0000335386, 0.0605988957; C, -0.009633352, 0.0000098052, 1.4637135621; C, 1.2422076922, 0.0000359727, 2.0962773463; C, 2.4124701004, 0.0000186057, 1.3452691864; C, 2.3529106335, -0.000024931, -0.0485851927; C, 1.1101958129, -0.000050727, -0.6821374411; N, -1.145639533, 0.0000270251, 2.2908979934; C, -2.3327797823, 0.0000033349, 1.9142781719; C, -3.2499647415, -0.0000486471, 0.9628322619; C, -4.3427702909, -0.0000863673, 0.326188595; O, -5.3333053682, -0.0001242879, -0.3153973257; N, -3.3019484929, 0.0000664463, 3.6333166916; C, -2.982972336,

1.2294585171, 4.367353859; C, -2.9824395177, -1.2289287565, 4.3677828505; H, 1.2757803879, 0.0000702711, 3.1795398616; H, 3.372950383, 0.0000392037, 1.8486927497; H, 3.264718519, -0.0000383818, -0.6347476209; H, 1.054793041, -0.0000841994, -1.7653182084; H, -1.0288999794, -0.0000535193, -0.4360881937; H, -4.2682145915, -0.0001953086, 3.3190193293; H, -3.46086056, -1.2471445566, 5.3533465578; H, -1.8990788859, -1.2775020348, 4.4886275551; H, -3.311466098, -2.092221673, 3.7883758003; H, -1.8996392546, 1.2785146343, 4.4882566675; H, -3.4614615944, 1.2478426195, 5.3528814066; H, -3.3123111516, 2.0924077605, 3.7876126163.

TS12b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7304373 (hartree), -2124930.83199539 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.9808537938, 1.4301263543, 0.543523537; C, 1.6472113644, 1.0603118955, 0.589298758; C, 1.170375765, -0.1521994422, 0.0679254657; C, 2.1455115547, -0.9927817989, -0.4889376453; C, 3.485998733, -0.6583644553, -0.5604381228; C, 3.9033022919, 0.565614669, -0.040737837; F, 0.7648718987, 1.8819197203, 1.1966322419; N, -0.1474513141, -0.5870873299, 0.1463315444; C, -1.1691949696, 0.0953136525, -0.0713928157; C, -1.786790384, 1.1796592262, -0.4744054561; C, -2.5943562933, 2.099461218, -0.7906734162; O, -3.3175504648, 2.9764097144, -1.0994972883; F, 1.7418108141, -2.1809493961, -0.9920528487; N, -2.5927452543, -1.244575083, 0.357104217; C, -2.5033881644, -2.3512799751, -0.6024352149; C, -2.4683432738, -1.6614893056, 1.7571526574; H, 4.1789050875, -1.3520941304, -1.0190154179; H, 4.9487455328, 0.8436472076, -0.0877621362; H, 3.2761270263, 2.38144443, 0.9674421817; H, -3.4352782283, -0.6965899534, 0.2087948858; H, -3.2406175911, -3.1333239626, -0.3879775411; H, -1.49903818, -2.7731353793, -0.5422397472; H, -2.664556126, -1.9685627666, -1.6108839609; H, -1.4608661465, -2.0538660574, 1.9054511918; H, -3.200104833, -2.4350955815, 2.0164657726; H, -2.6087637653, -0.7970297801, 2.4071587493.

TS12c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2468412 (hartree), -1646049.216801 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.8651414913, 0.0001929843, -3.3519721192; C, -0.8018939147, 0.0001839673, -1.9659658741; C, 0.4632051011, -0.0001132014, -1.351596309; N, 1.604962754, -0.0003867198, -2.0523536843; C, 1.5213810892, -0.0003717534, -3.3835619134; C, 0.3190227203, -0.0000900287, -4.0870642136; N, 0.6290117896, -0.0001478161, 0.0361113659; C, -0.2615511935, 0.0000908471, 0.903486739; C, -1.5281908283, 0.0004253365, 1.2741802529; C, -2.5914136513, 0.0007042531, 1.9610292002; O, -3.6127991715, 0.000971887, 2.5496065286; N, 0.8293627672, -0.0001875753, 2.5669072364; C, 1.6303922945, -1.2286490878, 2.5999427152; C, 1.6313002907, 1.2276865796, 2.59975399; H, 2.4687177758, -0.0005980487, -3.9162598292; H, 0.3148895242, -0.0000935411, -5.1702168471; H, -1.8276362993, 0.0004184851, -3.8518346489; H, -1.6988131367, 0.0003995484, -1.3600870506; H, 0.1204998338, 0.0001287439, 3.294758885; H, 2.30780971, -1.2466676924, 3.4610012036; H, 2.212996447, -1.273991246, 1.6781010643; H, 0.9668472314, -2.0932016845, 2.6426231504; H, 2.21393052, 1.2724549167, 1.6779014676; H, 2.308733472, 1.2453347416, 3.4608077214; H, 0.968394619, 2.0927360798, 2.6423034198.

TS12d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2430971 (hartree), -1646039.39136631 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.9167165974, 0.0001499233, -3.3556514195; C, -0.8519757072, 0.000126945, -1.9671226889; C, 0.4100140866,

0.0000300164, -1.3584953532; C, 1.5386034294, -0.0000461116, -2.1941549048; N, 1.478853794, -0.0000305251, -3.523209196; C, 0.2669991713, 0.0000697822, -4.0910284468; N, 0.6316509491, 0.0000256302, 0.0248861234; C, -0.2478980975, -0.0000337269, 0.9045847066; C, -1.5025250056, -0.0001573335, 1.3033247836; C, -2.560194967, -0.0002525801, 1.9993726156; O, -3.5735466664, -0.0003453678, 2.6000760363; N, 0.8843380462, 0.0001424076, 2.5785750098; C, 1.6826791027, -1.2285528387, 2.6147874722; C, 1.6828041934, 1.2287628541, 2.6144450412; H, 2.5262584438, -0.0001251368, -1.7411397803; H, 0.2446745259, 0.0000864424, -5.1766713203; H, -1.87423245, 0.0002292066, -3.8638440767; H, -1.7506768841, 0.0001863284, -1.3624919705; H, 0.1749820597, 0.0002779918, 3.3057053416; H, 2.3584881087, -1.2500059349, 3.4775399238; H, 2.2696584724, -1.2788705873, 1.6960383077; H, 1.0179880899, -2.0923377377, 2.6549208443; H, 2.2696745956, 1.2788270747, 1.6956122358; H, 2.3587166442, 1.2503285681, 3.4771142873; H, 1.0182045474, 2.0926225576, 2.6544735202.

TS12e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2441043 (hartree), -1646042.0345056 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.8888948853, -0.0000311851, -3.3478511312; C, -0.8238466918, -0.0000181559, -1.9580575531; C, 0.438527079, 0.0000095251, -1.3472403997; C, 1.5622071156, 0.0000248729, -2.183179147; C, 1.377913546, 0.0000101606, -3.5605251216; N, 0.1785901122, -0.0000178951, -4.1540822681; N, 0.6492900295, 0.0000233794, 0.0369497335; C, -0.2400285174, 0.0000117516, 0.9100558431; C, -1.4967291741, -0.0000028488, 1.2966766071; C, -2.5653427978, -0.0000139425, 1.9765427326; O, -3.5863308082, -0.0000243042, 2.5623554572; N, 0.8713351394, 0.0000133154, 2.5874413011; C, 1.6696727197, -1.2288565226, 2.6322773702; C, 1.6696865675, 1.2288705123, 2.6322729342; H, 2.5559747683, 0.0000474548, -1.7521388369; H, 2.2392440399, 0.000021415, -4.2228856512; H, -1.8575524075, -

0.0000534984, -3.8402543046; H, -1.7288919636, -0.0000297419, -1.3644596504; H, 0.1548325166, 0.0000168299, 3.3076653531; H, 2.3360946597, -1.2490050069, 3.5021045087; H, 2.2658881587, -1.2789654444, 1.7195338971; H, 1.0047631917, -2.0926933376, 2.6659890543; H, 2.2658949741, 1.2789732377, 1.7195231596; H, 2.336114863, 1.2490110513, 3.502095211; H, 1.0047869299, 2.0927148696, 2.6659894288.

Int2a

Optimised geometry: Program version = IA64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.2055949 (hartree), -1603953.06075163 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.0150009273, -0.0000394885, 0.0138280898; C, -0.006155848, -0.0000328861, 1.4064302583; C, 1.2157575615, -0.0000000488, 2.1044125744; C, 2.4114928217, 0.0000255299, 1.3630997428; C, 2.3925827934, 0.0000180736, -0.0258805858; C, 1.1761723556, -0.0000144371, -0.7106656665; N, 1.3565481415, 0.0000110716, 3.4970419346; C, 0.3872940571, -0.0000185174, 4.332178781; C, -0.9689783485, -0.0000693811, 4.3716164564; C, -2.1411950428, -0.0000990101, 4.8402901703; O, -3.2685098678, -0.0001308221, 5.2101499839; N, 1.020310442, 0.0000000443, 5.82182444; C, 1.8063897718, -1.2390353601, 6.0731196838; C, 1.8064169804, 1.2390230318, 6.0730933241; H, 3.3503684333, 0.000051077, 1.9051971874; H, 3.3271617104, 0.0000378152, -0.5763208295; H, 1.1577066044, -0.0000200945, -1.7946434009; H, -0.965454124, -0.0000647573, -0.5090973937; H, -0.9363424083, -0.0000531876, 1.9582003667; H, 0.1910980235, 0.0000142474, 6.4162557971; H, 2.1965849651, -1.227370914, 7.0921008378; H, 2.6156434389, -1.2679303515, 5.3470856468; H, 1.1526327613, -2.0981949986, 5.928697195; H, 2.6156509518, 1.267901097, 5.3470370053; H, 2.1966381155, 1.2273558724, 7.0920645245; H, 1.1526712225, 2.0981935939, 5.9286843193.

Int2b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7379845 (hartree), -2124950.63769521 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.6197482639, 0.0447086008, 0.1066587139; C, -2.794766726, 0.8383882415, 0.8998321504; C, -1.4353144588, 0.5772796531, 0.923223123; C, -0.8324656053, -0.4510482639, 0.1840144609; C, -1.7141017778, -1.2256394977, -0.5827512402; C, -3.0780939565, -0.9993337404, -0.6410561115; F, -0.643702246, 1.3254114004, 1.7283465057; N, 0.5176240832, -0.7799453969, 0.2606531569; C, 1.4265497552, 0.0709129751, -0.0721186534; N, 2.8353878829, -0.5673869877, 0.1806512329; C, 3.0504520029, -1.7754916726, -0.668950681; F, -1.1907561922, -2.2405899907, -1.3121264675; C, 1.563856468, 1.3216828872, -0.5995185935; C, 0.9033856151, 2.3363764525, -1.0102793556; O, 0.4186410769, 3.3285708667, -1.4151532116; C, 3.062650768, -0.8328533088, 1.6307504004; H, -3.6923720275, -1.6327718858, -1.2682425188; H, -4.6844782774, 0.2387252425, 0.0715050749; H, -3.1852938445, 1.6517576049, 1.4980082494; H, 3.4581660213, 0.1821161535, -0.1298820996; H, 4.0746331502, -1.2128799761, 1.775132605; H, 2.3227032014, -1.5603718014, 1.9557641258; H, 2.9254472608, 0.1005179212, 2.1749138397; H, 2.2925482734, -2.508051817, -0.402331988; H, 4.0541603812, -2.1650727885, -0.4961197177; H, 2.9299765011, -1.4844955422, -1.7114582309.

Int2c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2501744 (hartree), -1646057.96393353 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1577785717, -0.0000198905, -2.4788622481; C, -3.1533318335, 0.0000135466, -1.0861877459; C, -1.9416288931, 0.0000049953, -0.4087279507; C, -0.7466481254, -0.0000378443, -1.1549441852; N, -0.7508489794,

-0.0000711023, -2.5015098701; C, -1.9250685729, -0.0000614338, -3.1298175701; N, 0.5305098292, -0.000051784, -0.6006513118; C, 0.7977986875, -0.0000085866, 0.6504674589; N, 2.4079402927, -0.0000314262, 0.7961985792; C, 2.9953832787, 1.2383885595, 0.2123601893; C, 0.1833542243, 0.0000643197, 1.8591951503; C, 0.0495340617, 0.000095972, 3.115631315; O, -0.1547223854, 0.0001300167, 4.2830942535; C, 2.9953807627, -1.2384113727, 0.2122741116; H, -1.8800267753, -0.0000886094, -4.2162115954; H, -4.0810692051, -0.0000143226, -3.0455911188; H, -4.0844244274, 0.0000462688, -0.5295766484; H, -1.9027741022, 0.0000314727, 0.6718791981; H, 2.5503950469, -0.0000641476, 1.8063128539; H, 4.0793478325, -1.2227438024, 0.3350552318; H, 2.7215516565, -1.2646509485, -0.8402616194; H, 2.5693448774, -2.0992974597, 0.7259684583; H, 2.7216086601, 1.2646715628, -0.840188783; H, 4.0793447131, 1.2227395391, 0.3351933327; H, 2.5693027003, 2.099240909, 0.7260737312.

Int2d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2472733 (hartree), -1646050.35073715 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1887952882, -0.0000009629, -2.4288030699; C, -3.1805243736, 0.0000022649, -1.0366381358; C, -1.9650231409, 0.0000019549, -0.3598747641; C, -0.7785859757, -0.0000016596, -1.1111706728; C, -0.9088482482, -0.0000047314, -2.514176395; N, -2.0684699864, -0.0000044236, -3.1634862728; N, 0.5251342394, -0.0000025768, -0.6152792934; C, 0.8252488326, 0.0000001009, 0.630819684; N, 2.4296812639, -0.0000021336, 0.7536791022; C, 3.0166501548, 1.2397291493, 0.1713001826; C, 0.2237663502, 0.0000042422, 1.8471376704; C, 0.1149222103, 0.0000077661, 3.1062326773; O, -0.0670746383, 0.0000111851, 4.2773493476; C, 3.0166464239, -1.2397377458, 0.1713056513; H, -0.0042706934, -0.0000075637, -3.1169683159; H, -4.1251569357, -0.0000007785, -2.9789683427; H, -4.1153761136, 0.0000050108, -0.4873710154; H, -1.9257115366, 0.000004427, 0.7212114803; H, 2.5792729935, -

0.0000001325, 1.76298573; H, 4.1000759436, -1.2268095312, 0.2988094991; H, 2.7492924264, -1.267406177, -0.8824031669; H, 2.5859642689, -2.0992668337, 0.6831657938; H, 2.7492964159, 1.2673936235, -0.88240881; H, 4.100079618, 1.2267983493, 0.29880425; H, 2.5859704298, 2.0992617927, 0.6831563971.

Int2e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2480331 (hartree), -1646052.34463829 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, -3.058436534, 0.000000692, -2.6779534128; C, -3.0513024509, 0.0000006059, -1.3406633388; C, -1.9018826957, 0.0000003901, -0.5551671881; C, -0.6487873147, 0.0000002821, -1.1919368448; C, -0.6528184693, 0.0000003934, -2.5972561271; C, -1.8614456283, 0.0000005815, -3.2790998387; N, 0.597573085, 0.0000001035, -0.566921458; C, 0.7695934996, -0.0000001451, 0.7054626116; N, 2.3560090385, -0.0000003098, 0.9851381897; C, 2.9967790487, 1.2398636358, 0.4628081786; C, 0.0564761068, -0.0000003436, 1.8560208442; C, -0.1913336383, -0.0000006207, 3.0954769675; O, -0.4983496889, -0.0000008639, 4.2390229902; C, 2.9967788459, -1.2398641832, 0.4628077547; H, 0.2888613849, 0.0000003198, -3.1334161753; H, -1.8724121529, 0.0000006541, -4.3658549597; H, -4.0264165038, 0.0000007117, -0.8606209128; H, -1.9764850686, 0.0000003203, 0.5232108542; H, 2.4063454969, -0.000000486, 2.0043018402; H, 4.0625476304, -1.2267633571, 0.6954368843; H, 2.8333161749, -1.2674850484, -0.6119142722; H, 2.5184065045, -2.0994747051, 0.9302936241; H, 2.8333163794, 1.267484907, -0.6119138365; H, 4.0625478316, 1.2267625447, 0.6954373023; H, 2.5184068854, 2.0994740739, 0.9302943837.

TS22a

Optimised geometry: Program version = IA64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.1765925 (hartree), -1603876.95135631 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.0120414868, -0.0126767679, 0.0182237197; N, 0.0096071531, 0.0119557598, 1.2880680422; N, 1.3487937229, 0.0000652825, -0.7038001549; C, -0.8383319358, -0.0952013437, -1.1180068655; C, -2.0921008405, -0.1789851199, -1.4317997604; O, -3.1802726351, -0.2498375094, -1.8516195982; C, -1.1685558611, 0.0406752404, 2.0529833463; C, -1.1904332579, -0.7008712656, 3.2437637876; C, -2.3155912157, -0.6925193563, 4.0606782167; C, -3.4283221616, 0.0780844617, 3.7209613494; C, -3.402241873, 0.8405527659, 2.5545181907; C, -2.2857702663, 0.8231690945, 1.7222663605; C, 2.069475828, 1.2776681157, -0.5575812946; C, 2.1818967415, -1.1778752039, -0.4022291341; H, -0.3144452506, -1.2815545632, 3.5083735797; H, -2.3210235468, -1.2822001094, 4.9708301666; H, -4.3017366981, 0.0907531348, 4.3626560002; H, -4.2556268418, 1.4542494782, 2.2878392394; H, -2.2699478049, 1.4354858302, 0.8290082451; H, 2.3645115762, 1.4311326669, 0.483832856; H, 1.412243951, 2.0910102326, -0.8686738656; H, 2.9546256912, 1.2647232498, -1.1955228009; H, 3.066346504, -1.1627809682, -1.0409818255; H, 1.6035013055, -2.0799630095, -0.6064866477; H, 2.4813205402, -1.1728973094, 0.6488517818; H, 0.4590587165, -0.0922830041, -1.6832863953.

TS22b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7081255 (hartree), -2124872.28037185 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.8308675054, 0.8138469507, 0.8855361461; C, 1.4672525123, 0.5745684831, 0.9117535215; C, 0.8608740407, -0.5067657656, 0.2572314399; C, 1.7374390763, -1.3565243747, -0.431731969; C, 3.1045992255, -1.1510492168, -0.4927523738; C, 3.6523914256, -0.0558741032, 0.1730052006; F, 0.6736431344, 1.4060855824, 1.6287182724; N, -0.4965050889, -0.8145013112, 0.3563289268; C, -1.3906026605, -

0.0050457135, -0.0515031277; C, -1.5586725128, 1.2333671343, -0.714181431; C, -0.8397476335, 2.2011031055, -1.1937452628; O, -0.3154502986, 3.1321779437, -1.6610665948; F, 1.2075096216, -2.4195256663, -1.0771779908; N, -2.8450268427, -0.3776082459, 0.1284058383; C, -3.2285550081, -1.5950454108, -0.6112166583; C, -3.2587260144, -0.397449655, 1.5443234691; H, 3.7173486448, -1.8429836444, -1.0562843038; H, 4.7203295463, 0.1191172678, 0.1363832958; H, 3.2264771136, 1.6690705308, 1.4183414697; H, -2.8865302124, 0.7916584105, -0.5074243578; H, -4.3077192396, -1.7335541838, -0.5321707281; H, -2.7090543946, -2.4664704087, -0.2050805469; H, -2.9547294807, -1.471411434, -1.6597610105; H, -2.7561410665, -1.2094453935, 2.0763085699; H, -4.3400197273, -0.5327560912, 1.597241093; H, -2.9887298172, 0.5542904488, 2.0036596591.

TS22c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2198836 (hartree), -1645978.47346129 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.9918806398, 0.4077413985, 0.9164990607; C, 1.6124449969, 0.2551209466, 0.9379372598; C, 1.0270561087, -0.7066939513, 0.0970513773; N, 1.7495465135, -1.4879596641, -0.7141080832; C, 3.0733015364, -1.3153422805, -0.7319251601; C, 3.7479815152, -0.3894334898, 0.0594358367; N, -0.351792402, -0.9587308789, 0.1106113644; C, -1.2104519051, -0.0318840351, -0.0046609116; C, -1.3400672256, 1.3661611193, -0.2238579995; C, -0.6072848009, 2.4186987832, -0.40902257; O, -0.067859838, 3.4405730513, -0.5787360244; N, -2.6825175508, -0.3908876502, 0.0525587549; C, -3.0974696684, -1.2722189986, -1.0557147304; C, -3.1071012948, -0.8796376232, 1.3768975571; H, 3.6236390198, -1.9599038141, -1.4122383402; H, 4.8263610354, -0.3027176462, 0.0080440412; H, 3.469242975, 1.1397213828, 1.5586181888; H, 0.9941873588, 0.85242809, 1.596411678; H, -2.6802951559, 0.9238487974, -0.1594532078; H, -4.180624048, -1.3984790125, -1.0234306844; H, -2.6034711223, -2.2434440739, -0.9735037099; H, -2.8145165936, -0.8062855066, -2.0005179254; H, -2.6203526851,

-1.831564412, 1.6050251221; H, -4.1905624152, -1.0076599721, 1.3798627829; H, -2.8291250032, -0.1425521057, 2.1317976793.

TS22d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2167347 (hartree), -1645970.20997707 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.0182161454, 0.3777391431, -2.275690925; C, -2.975268104, 0.5753270489, -0.8980701234; C, -1.7417132489, 0.5881850749, -0.2556432216; C, -0.5814832587, 0.4044562832, -1.0183648054; C, -0.7413462194, 0.2427910414, -2.4060635794; N, -1.9196348141, 0.2160004612, -3.0231303441; N, 0.724566537, 0.4383029354, -0.5159758909; C, 1.0516691286, -0.0468250457, 0.612917903; N, 2.4942988428, 0.0809963064, 1.0649872714; C, 2.8858730014, 1.4719835679, 1.3582375931; C, 0.5469887744, -0.7760349436, 1.722347827; C, -0.5391267241, -1.3299661152, 2.1597348145; O, -1.4457800766, -1.8612817026, 2.6696167475; C, 3.4433373548, -0.6180757444, 0.1789116139; H, 0.1449075341, 0.1259901145, -3.0234120767; H, -3.9669567889, 0.3576533087, -2.8034581405; H, -3.8919518672, 0.7184509357, -0.3377161798; H, -1.6795556363, 0.7624250156, 0.8114726133; H, 1.9113741941, -0.6133528084, 2.0406176451; H, 4.437194833, -0.5888075262, 0.6278833003; H, 3.4652318168, -0.1440007683, -0.8055078768; H, 3.125791299, -1.656044774, 0.0707710981; H, 2.8769290695, 2.0712651046, 0.4439518335; H, 3.8859103389, 1.4771353111, 1.794397776; H, 2.1784645083, 1.8949599223, 2.0729961919.

TS22e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2184256 (hartree), -1645974.64731248 (kJ mol^{-1}). Structure definition (3D

Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.6700145972, 0.6221829674, -3.0141702059; C, -0.6384724535, 0.6333211115, -1.6227281688; C, 0.5950064008, 0.4837306179, -0.9730090035; C, 1.7324979595, 0.3477080457, -1.7797602122; C, 1.5828131399, 0.3360204227, -3.1611212068; N, 0.4083669964, 0.4706435421, -3.7891170701; N, 0.7568795356, 0.5359349815, 0.4151512731; C, -0.0246314656, -0.0606768428, 1.2227207227; C, -1.1272470749, -0.9506044592, 1.2759755352; C, -1.9226943263, -1.6095589391, 0.4918174483; O, -2.7053903218, -2.2461736919, -0.0937426618; N, 0.2037655044, 0.1087389861, 2.7121892399; C, 1.5014176736, -0.4266345103, 3.1643460615; C, -0.0578964928, 1.4814028459, 3.1834160814; H, 2.7098437413, 0.2512321623, -1.3227259017; H, 2.4543884108, 0.218804351, -3.7993642236; H, -1.6177046037, 0.7414448614, -3.5322500036; H, -1.5519682815, 0.7793073574, -1.0599215372; H, -0.8255927366, -0.7300288111, 2.63895587; H, 1.5428698665, -0.3853433792, 4.2536816254; H, 2.3229109397, 0.1546452519, 2.7382124375; H, 1.5875550536, -1.4640842018, 2.8384238061; H, 0.670218551, 2.1760798872, 2.7564343941; H, 0.0043633052, 1.5025909491, 4.2723695092; H, -1.0615185068, 1.776170981, 2.8736389076.

TS13a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4283031 (hartree), -1958810.53998659 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, -1.1777548233, 0.1625592124, 0.1377974759; C, -0.2834537154, -0.6928423584, 0.0484813521; C, 0.6937565901, -1.4824643238, -0.0359439585; C, 1.8925248007, -2.0309828215, -0.1047898869; O, 2.5730789005, -2.994572785, -0.231493952; C, -2.5660375351, -0.0343988305, 0.0807430313; C, -3.3958891024, 1.085525164, 0.2218576414; C, -4.7792857478, 0.9457961622, 0.1712117904; C, -5.3554637953, -0.3097411009, -0.0206704803; C, -4.53152813, -1.4275429409, -0.1615642166; C, -3.147863929, -1.2975225482, -0.1120720192; N, 3.1466562723, -0.5065057006, 0.1443575247; C, 3.6912427043, -

0.6146411063, 1.5021640945; C, 4.1721620071, -0.5854145609, -0.898358932; H, -2.9389895186, 2.0567352026, 0.3716358608; H, -5.4097591396, 1.8211510304, 0.2822972876; H, -6.4332660895, -0.4171117413, -0.0598164615; H, -4.9696022487, -2.4084410512, -0.3111609038; H, -2.5092424015, -2.1670159811, -0.221888326; H, 2.5883382529, 0.3581128252, 0.0474823132; H, 4.4416041844, 0.1605385206, 1.6987805686; H, 4.1573351489, -1.5946623317, 1.6255051614; H, 2.8806562357, -0.5167649998, 2.22557833; H, 4.5992547746, -1.5905464814, -0.9020663682; H, 4.9745485719, 0.1433892304, -0.732122808; H, 3.715773792, -0.397235877, -1.8711578981; N, 1.516606265, 2.10932285, -0.1231992539; C, 1.8320023871, 3.1160332614, 0.8918205218; C, 1.5726717831, 2.6476198467, -1.4843562709; H, 0.5789726832, 1.7486103597, 0.0448840965; H, 1.2056859672, 4.01902496, 0.8169374033; H, 2.8765763773, 3.4271057175, 0.7927172484; H, 1.6991963282, 2.6892903128, 1.8884144975; H, 2.601158157, 2.9311861828, -1.7283045997; H, 0.9373698029, 3.5361425398, -1.62471438; H, 1.2521740177, 1.8828962714, -2.1948756362.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.436347 (hartree), -1958831.64914877 (kJ mol^{-1}).

TS13b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9584917 (hartree), -2479802.34096752 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -2.9424150846, -1.3309345034, -0.0349433691; C, -2.2351739192, -0.117394713, 0.0158633148; C, -3.0342224416, 1.0379464285, 0.0378946646; C, -4.4165932372, 1.008366613, 0.0113224704; C, -5.0649239485, -0.2245981526, -0.038686774; C, -4.3236315793, -1.4044028409, -0.0618962043; N, -0.8618611201, 0.0149377073, 0.0492097711; C, 0.0497193205, -0.8308125739, 0.0095860858; C, 1.0746991353, -1.5541155763, -0.0255292724; C, 2.3061435372, -2.0302214417, -0.0490196476; O, 3.0493797262, -

2.9502807026, -0.1165086822; N, 3.463375799, -0.4142201218, 0.1307694746; C, 4.4426344892, -0.4362753924, -0.9584216182; C, 4.0767613248, -0.4703048691, 1.4616530129; N, 1.6804148573, 2.105215175, -0.0813781148; C, 1.756904497, 2.7242468691, -1.4070360696; C, 1.9094475783, 3.0680415324, 0.9981313581; F, -2.4093149849, 2.2359958766, 0.0862267771; H, -4.9638782174, 1.9420614171, 0.0303263918; H, -6.1466581257, -0.2659707792, -0.0596521329; H, -4.7966746465, -2.3774479229, -0.1004678097; F, -2.2260956325, -2.4752960278, -0.0568506236; H, 2.8452417899, 0.4114866711, 0.0523349023; H, 4.7900554588, 0.3488987726, 1.6124217466; H, 4.602971965, -1.4206684399, 1.5750641965; H, 3.2972200722, -0.4068755966, 2.2222347713; H, 4.9464357037, -1.4052848005, -0.9656460315; H, 5.1934412801, 0.3547549419, -0.8431867236; H, 3.9286215945, -0.3023946363, -1.9113150454; H, 0.7533802259, 1.6982276582, 0.0313336191; H, 1.2385258705, 3.939723179, 0.9500878746; H, 2.9392831898, 3.4359934457, 0.9537865029; H, 1.7657386811, 2.5794673148, 1.9643895988; H, 2.7778627388, 3.0703497202, -1.596224409; H, 1.0824109385, 3.5870187279, -1.51999575; H, 1.5000744447, 1.987829707, -2.1715232509.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9669597 (hartree), -2479824.56307188 (kJ mol^{-1}).

TS13c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4726929 (hartree), -2000914.94534926 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1409988084, -1.3461666697, -0.0616984509; C, -2.5407357769, -0.0794168337, 0.0640699925; N, -3.2516567719, 1.0500159688, 0.1540659452; C, -4.5828944637, 0.9526042692, 0.1220329638; C, -5.2729234385, -0.2502033585, 0.0015767028; C, -4.5241738779, -1.4239085595, -0.0920478238; N, -1.1554675848, 0.0811296901, 0.1040552962; C, -0.2673764236, -0.7789514037, 0.0247012885; C, 0.7062444094, -

1.5741173272, -0.0513617081; C, 1.9294764627, -2.0644345633, -0.1164868592; O, 2.6691587588, -2.9807950697, -0.2299311538; N, 3.1227664192, -0.4428168517, 0.1112610568; C, 4.1215916632, -0.4649891856, -0.9585202143; C, 3.707919962, -0.5290924679, 1.4524806641; N, 1.3878346439, 2.121138315, -0.0817212723; C, 1.4430788001, 2.7255473804, -1.4150141917; C, 1.6822620107, 3.0848959748, 0.9806452035; H, -5.1256585816, 1.89111877, 0.1974478389; H, -6.3556671632, -0.2649632885, -0.0178724986; H, -5.0134382377, -2.3871162038, -0.1879055976; H, -2.5233515341, -2.2336747844, -0.1320414718; H, 2.5195982165, 0.3934263597, 0.034215984; H, 4.4288681638, 0.2777635376, 1.6331071332; H, 4.2206326231, -1.4875779526, 1.5614366628; H, 2.9143378805, -0.4681859226, 2.1986909648; H, 4.6039851911, -1.4449439678, -0.9774020163; H, 4.8889931782, 0.3055773621, -0.8140644544; H, 3.6298681098, -0.3001015727, -1.9183710061; H, 0.4519808787, 1.7452117892, 0.06317133; H, 1.0408395535, 3.9791665495, 0.9437532072; H, 2.722466605, 3.416599411, 0.9025235719; H, 1.5501095644, 2.6105677941, 1.9556090088; H, 2.4684219429, 3.0359812439, -1.6395546194; H, 0.7939628611, 3.6091247548, -1.5154781131; H, 1.1376206193, 1.9915132903, -2.163709278.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4818124 (hartree), -2000938.87714907 (kJ mol^{-1}).

TS13d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4684904 (hartree), -2000903.91696079 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1674373939, -1.3485364175, -0.1125492696; C, -2.5757791952, -0.0925930013, 0.0735228349; C, -3.4258959791, 1.0156908923, 0.2094549017; N, -4.7543045489, 0.939593109, 0.1710531605; C, -5.3057007928, -0.2659925243, -0.0070831006; C, -4.553418816, -1.4310695145, -0.1523944893; N, -1.1952808829,

0.1225468304, 0.1306174026; C, -0.2890204892, -0.7194601539, 0.0396396495; C, 0.696986618, -1.4972094862, -0.0457777027; C, 1.8898821751, -2.0478334849, -0.1239378437; O, 2.5984546805, -2.9849352159, -0.2543673531; N, 3.1630569116, -0.4593547926, 0.1352194568; C, 4.1827541859, -0.5259186493, -0.9118502418; C, 3.712755477, -0.5705681818, 1.4889120827; N, 1.4817735683, 2.1436726643, -0.1049170192; C, 1.5420171645, 2.7145690083, -1.4526213492; C, 1.7865351105, 3.1277498374, 0.9356074939; H, -2.9885921154, 1.9994744917, 0.3555151225; H, -6.390616288, -0.3003485495, -0.0344732673; H, -5.0474119905, -2.3854904528, -0.2946228457; H, -2.5476162709, -2.2317399931, -0.2220799687; H, 2.5945356245, 0.3974086396, 0.0443161041; H, 4.460857512, 0.2066187915, 1.6900709467; H, 4.185644982, -1.5483184026, 1.6077891186; H, 2.9053531434, -0.4810160448, 2.2172851327; H, 4.6181100034, -1.5279367672, -0.9246883858; H, 4.9840550104, 0.2058075234, -0.7484884627; H, 3.7215399287, -0.3354911388, -1.8821409005; H, 0.5461098753, 1.7738870575, 0.0504877871; H, 1.1559054482, 4.0289304365, 0.8794555765; H, 2.8299360101, 3.446031244, 0.8487172002; H, 1.6517919626, 2.6764685314, 1.9210519051; H, 2.5701927425, 3.0099336444, -1.6831132169; H, 0.9021359659, 3.6022213388, -1.576031955; H, 1.2316472862, 1.9648667537, -2.1834598645.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4777821 (hartree), -2000928.30065554 (kJ mol^{-1}).

TS13e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4703811 (hartree), -2000908.8786203 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1799518262, -1.28631054, -0.1175488316; C, -2.5740556422, -0.0372918956, 0.0828332466; C, -3.4129483878, 1.0729335495, 0.2311764542; C, -4.7894494144, 0.8865243312, 0.173359985; N, -5.3784748021, -

0.2992950279, -0.0177797008; C, -4.5673845655, -1.3549019009, -0.1584066908; N, -1.1914430124, 0.1505142232, 0.1395340106; C, -0.3024030368, -0.7102386052, 0.039951082; C, 0.6703492196, -1.5018519491, -0.0524412735; C, 1.8487460761, -2.080020025, -0.1360390039; O, 2.545722713, -3.0219945406, -0.2733016895; N, 3.1657086451, -0.4993058364, 0.1390376785; C, 4.1909364247, -0.5847036498, -0.9005728875; C, 3.7025004926, -0.6244544475, 1.4962110586; N, 1.5226623436, 2.13328131, -0.1077926079; C, 1.5858618529, 2.6920227533, -1.4603284004; C, 1.8501877687, 3.1195970931, 0.9234431845; H, -2.9878417814, 2.0565614911, 0.3891780728; H, -5.4554816324, 1.7375425674, 0.286931825; H, -5.0551570354, -2.3135571932, -0.3131134966; H, -2.5786385565, -2.1798774826, -0.2386492533; H, 2.614299441, 0.3675945308, 0.0457639066; H, 4.4639771496, 0.13751843, 1.7064924919; H, 4.1563875457, -1.6110967307, 1.6168326472; H, 2.8916790911, -0.5217606212, 2.21915319; H, 4.6056003871, -1.595617958, -0.9137519991; H, 5.0073952959, 0.1288521895, -0.7303713604; H, 3.741385713, -0.3819884515, -1.8739112408; H, 0.5822275397, 1.7796449176, 0.0554804454; H, 1.235665862, 4.031735487, 0.8635149677; H, 2.8985876976, 3.4185140915, 0.8288260402; H, 1.7128014965, 2.6783632996, 1.9130664917; H, 2.6178436957, 2.9673611798, -1.6982843171; H, 0.9611844658, 3.5899519786, -1.5880476427; H, 1.2587959303, 1.9420236324, -2.1835204543.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4796668 (hartree), -2000933.24656958 (kJ mol^{-1}).

Int3a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.429633 (hartree), -1958814.02996965 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, 1.1911957837, 0.2756949151, -0.0008279569; C, 0.2904484891, -0.5942197511, 0.0000577466; C, -0.6919952445, -

1.3720741357, 0.0008668582; C, -1.9502447656, -1.8627043774, 0.0015911284; O, -2.5108747167, -2.9354234122, 0.0026546521; C, 2.5713247291, 0.0228995057, -0.0006586489; C, 3.4400672804, 1.123646921, -0.0020492764; C, 4.8185001222, 0.9353545668, -0.001922356; C, 5.3560249729, -0.3519536135, -0.0003983435; C, 4.4957219125, -1.4512482451, 0.0009947489; C, 3.116601778, -1.2719709673, 0.0008714329; N, -3.0317968758, -0.5922203363, 0.0007031175; C, -3.8552982553, -0.6592508543, -1.2293155846; C, -3.8553118952, -0.6574981728, 1.2308039249; H, 3.0141595916, 2.120412868, -0.0032266867; H, 5.4763082758, 1.7978631766, -0.0030174192; H, 6.4301421408, -0.4974411879, -0.0002955043; H, 4.9020394751, -2.4571154594, 0.0021915485; H, 2.4510213448, -2.128208312, 0.0019648836; H, -2.4838435596, 0.3032251898, 0.0000692541; H, -4.5949217354, 0.1440273262, -1.2266733286; H, -4.3520626094, -1.6281562456, -1.2641281931; H, -3.2027687936, -0.5556074489, -2.0958796954; H, -4.3520561148, -1.6263615806, 1.2670016508; H, -4.5949375111, 0.1457726692, 1.2269940767; H, -3.2027998205, -0.5526018386, 2.0972305813; N, -1.5924792594, 2.0179690918, -0.000950936; C, -1.8201325379, 2.8017904731, -1.2197211385; C, -1.8193035443, 2.8024602965, 1.2175418982; H, -0.6241193938, 1.6951722998, -0.0011863801; H, -1.2314780491, 3.7307940338, -1.2472742694; H, -2.8774647359, 3.0736799941, -1.2956022542; H, -1.5556450769, 2.2047073106, -2.0948569449; H, -2.8765973067, 3.0743294236, 1.2940307375; H, -1.2306870438, 3.7315162181, 1.2441571406; H, -1.5541471318, 2.2058832909, 2.0928196737.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4419832 (hartree), -1958846.43991691 (kJ mol^{-1}).

Int3b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9599557 (hartree), -2479806.1828618 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.906504829, -

1.3277108338, 0.0219930606; C, 2.2363683148, -0.0916857632, -0.0236665863; C, 3.0797691145, 1.0334503896, -0.0544344486; C, 4.4603519777, 0.957341411, -0.0416839286; C, 5.0680449103, -0.2965588111, 0.003744458; C, 4.2848902176, -1.4486190209, 0.035895011; N, 0.8698980439, 0.0998398194, -0.0395447338; C, -0.0573608012, -0.7478160259, -0.0156890702; C, -1.097771419, -1.4379253608, 0.0044617743; C, -2.3930104598, -1.8260273816, 0.0134840521; N, -3.3679863272, -0.4743902668, -0.0478310113; C, -4.2690617298, -0.4684262405, 1.1279170655; O, -3.0361353776, -2.848771086, 0.0472678536; C, -4.1151571361, -0.4810583365, -1.3279186182; N, -1.738154796, 2.0096140605, 0.0461685544; C, -1.8294951722, 2.687748977, 1.3445099655; C, -1.9820641169, 2.9228101222, -1.0757577867; F, 2.499197995, 2.2558589262, -0.0980176771; H, 5.0382207495, 1.8723953553, -0.0674925094; H, 6.147875891, -0.3753265075, 0.0141242364; H, 4.7230803032, -2.4380902296, 0.0716647023; F, 2.1562999408, -2.4510214719, 0.0541399929; H, -2.7511039267, 0.3766381327, -0.0152155696; H, -4.7810458202, 0.3830087012, -1.3746750277; H, -4.6917992456, -1.4032278286, -1.3919864601; H, -3.4022291947, -0.4405441814, -2.1510917636; H, -4.8344472894, -1.3994230335, 1.1389510942; H, -4.9476016216, 0.3852209003, 1.0722657934; H, -3.666489363, -0.4002414544, 2.0333245039; H, -0.7950871894, 1.6290693875, -0.0452026425; H, -1.3239530618, 3.80386266, -1.0604345682; H, -3.0173214685, 3.2768848234, -1.0492468727; H, -1.8244522597, 2.3964227767, -2.0195555403; H, -2.8563104082, 3.0245728646, 1.51770878; H, -1.1696724174, 3.5646842137, 1.4142799424; H, -1.5564116961, 1.9921409759, 2.1406588749.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9727114 (hartree), -2479839.65694029 (kJ mol^{-1}).

Int3c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4746331 (hartree), -2000920.03690888 (kJ mol^{-1}). Structure definition (3D

Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.1030672842, -1.2991612718, -0.0000314892; C, 2.5493390908, -0.0031849123, -0.0000174777; N, 3.3100747843, 1.10013192, -0.0000130538; C, 4.6360601391, 0.9454143699, -0.0000223176; C, 5.2784374751, -0.2893350307, -0.0000363845; C, 4.4814349641, -1.4353616544, -0.0000410675; N, 1.1737111768, 0.2211847743, -0.0000076733; C, 0.2798132933, -0.6564739078, -0.0000070686; C, -0.6989482786, -1.4374738437, -0.0000046304; C, -1.9847189425, -1.8626341246, -0.0000043778; N, -2.9987367844, -0.5489104874, -0.0000008521; C, -3.8254723027, -0.5747644797, 1.2303219321; O, -2.5904547798, -2.9094100417, -0.0000068234; C, -3.8254434494, -0.5747396892, -1.2303437749; N, -1.4889384558, 2.0064575781, 0.0000406863; C, -1.7068528471, 2.7949700172, 1.2183446972; C, -1.7068940256, 2.7950383338, -1.2182115354; H, 5.2170882421, 1.8643166746, -0.0000182097; H, 6.3599014666, -0.3490943367, -0.0000434157; H, 4.9310528462, -2.4226025834, -0.0000520433; H, 2.4503888195, -2.1642048594, -0.0000348111; H, -2.4119301612, 0.3254224767, 0.0000144182; H, -4.5233361865, 0.2647409648, -1.2251834598; H, -4.3700668469, -1.5174466133, -1.2660995828; H, -3.1690079401, -0.5012909095, -2.0969835787; H, -4.3700931731, -1.5174739461, 1.2660478884; H, -4.5233676641, 0.2647139775, 1.2251601743; H, -3.1690576933, -0.5013292544, 2.0969787058; H, -0.5207879456, 1.6801884098, 0.0000161576; H, -1.1046450555, 3.7147543762, -1.2437602135; H, -2.7605985586, 3.0812872479, -1.2941482234; H, -1.4492624525, 2.1958541061, -2.0940105328; H, -2.7605548014, 3.0812146183, 1.2943330566; H, -1.1046026939, 3.7146843255, 1.2439244371; H, -1.4491914138, 2.1957363245, 2.094101036.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.488672 (hartree), -2000956.87841821 (kJ mol^{-1}).

Int3d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated

Energy E(HF) = -762.4706688 (hartree), -2000909.6336155 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1399538751, -1.2799913529, -0.0000815352; C, -2.5801480507, 0.0052513878, -0.0000482704; C, -3.4658541735, 1.0959067526, -0.0000802126; N, -4.791838105, 0.9794097904, -0.0001399484; C, -5.3097941024, -0.2544509692, -0.0001707474; C, -4.5235021927, -1.4058560243, -0.0001431215; N, -1.2082519156, 0.2731610965, 0.0000133663; C, -0.3019023582, -0.5939166285, 0.0000499638; C, 0.6824426418, -1.3665467829, 0.0000856159; C, 1.9442138109, -1.8554341174, 0.0001444137; N, 3.0191796676, -0.5958003012, 0.0002287714; C, 3.8440875605, -0.6617389899, -1.2302911525; O, 2.496318203, -2.932501025, 0.0001645984; C, 3.8436547978, -0.6615687857, 1.2310500673; N, 1.5961544948, 2.0111294103, -0.0001562005; C, 1.8305731164, 2.7938447347, -1.2192616267; C, 1.8307546657, 2.7943059502, 1.2186164735; H, -3.0560389697, 2.1023786771, -0.000055253; H, -6.39355916, -0.3227979875, -0.0002189385; H, -4.9901410312, -2.3845979714, -0.0001697493; H, -2.4955695643, -2.1524953544, -0.000058501; H, 2.4735794663, 0.3032131332, 0.0000757925; H, 4.5803865181, 0.1439868281, 1.2268118737; H, 4.3429374635, -1.6290422645, 1.265533374; H, 3.1910009314, -0.5589600674, 2.0975752072; H, 4.3433347547, -1.6292403145, -1.2644914735; H, 4.5808540266, 0.1437837725, -1.2258778667; H, 3.1917475649, -0.5591954472, -2.0970603556; H, 0.6242237534, 1.7001931883, -0.0000318278; H, 1.250043037, 3.7279060928, 1.2447959867; H, 2.8903693054, 3.0569448707, 1.2937234312; H, 1.5612142391, 2.2003538697, 2.0943170764; H, 2.8901765914, 3.056453982, -1.2946262118; H, 1.2498556427, 3.7274330774, -1.2457058732; H, 1.5608997701, 2.199559097, -2.094694608.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4850453 (hartree), -2000947.36106985 (kJ mol^{-1}).

Int3e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4729476 (hartree), -2000915.61374439 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.1333065418, -1.2501455291, -0.0007692439; C, 2.5791674666, 0.0402332228, 0.0006473845; C, 3.4730319855, 1.1196406875, 0.0021015886; C, 4.8392846099, 0.8659384808, 0.0020928874; N, 5.3765474209, -0.3599802575, 0.0007530743; C, 4.5159334409, -1.3861145683, -0.0006483268; N, 1.2089457446, 0.3038862539, 0.0006597661; C, 0.3087932463, -0.5731941075, -0.0002948358; C, -0.6715718599, -1.3479507002, -0.0011523658; C, -1.9299206631, -1.8501184518, -0.0019839888; N, -3.0163863569, -0.607182282, -0.0013533137; C, -3.841270205, -0.6835084558, 1.2292216306; O, -2.4657514524, -2.9344054148, -0.0030599359; C, -3.8399439292, -0.681161443, -1.2329642107; N, -1.6236580106, 2.0096569898, 0.0015646558; C, -1.8671626109, 2.7887167252, 1.2214282225; C, -1.8673126721, 2.7911658035, -1.2166941949; H, 3.0932360334, 2.1343520274, 0.0032232894; H, 5.542764759, 1.6945180705, 0.0032255052; H, 4.9591351526, -2.3785733496, -0.0017401063; H, 2.4928457072, -2.1246702465, -0.0019483162; H, -2.4812852077, 0.2990740792, -0.0002182985; H, -4.5837868369, 0.1176690888, -1.2285126319; H, -4.3303383042, -1.6531106262, -1.267490958; H, -3.1879340279, -0.5724428389, -2.0992164669; H, -4.3315394302, -1.655599155, 1.2614580169; H, -4.5852431527, 0.115204326, 1.2254024129; H, -3.1902220913, -0.5762527677, 2.0963791296; H, -0.648151529, 1.710027456, 0.0012270011; H, -1.2976314647, 3.7315240111, -1.2416322281; H, -2.9298659984, 3.0415085666, -1.291655688; H, -1.5906060456, 2.2013187702, -2.0929138211; H, -2.9296988464, 3.0389443896, 1.2970009756; H, -1.2974337762, 3.7289924108, 1.2481945125; H, -1.5903870123, 2.1970841917, 2.0964206008.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4877683 (hartree), -2000954.50688825 (kJ mol^{-1}).

TS23a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4187187 (hartree), -1958785.38817541 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, -1.1180814939, 0.2018463579, -0.4305628674; C, -0.2230584534, -0.677855607, -0.2473772387; C, 0.7842135634, -1.389776997, -0.0718654939; C, 2.1205023198, -1.6316201, 0.1796885969; O, 2.7158373019, -2.5798582356, 0.6598769; C, -2.4903637778, -0.0019729094, -0.2363266488; C, -3.3574776142, 1.0804770534, -0.4539822201; C, -4.729668608, 0.9374422028, -0.275565873; C, -5.2684442275, -0.2867928851, 0.1219461763; C, -4.4124599087, -1.3682573127, 0.3369795656; C, -3.0392062851, -1.2339550321, 0.1615163923; N, 2.9678271302, -0.4077165101, -0.2510433231; C, 4.257165087, -0.3756015455, 0.4679313338; C, 3.1800290505, -0.4389661163, -1.7176087848; H, -2.9350480512, 2.0278532996, -0.7702719249; H, -5.3827563595, 1.7859967607, -0.450211682; H, -6.3378834768, -0.3976896479, 0.2591435375; H, -4.8180081077, -2.3267339858, 0.6437273357; H, -2.3792000178, -2.0783100848, 0.328404658; H, 2.1977997009, 0.7072251201, 0.0197761421; H, 4.807849947, 0.520939493, 0.1708670345; H, 4.8545672257, -1.2624306795, 0.2469049012; H, 4.075641887, -0.3514821493, 1.5425065018; H, 3.7328066384, -1.3374318278, -2.0097170931; H, 3.7509061816, 0.441447582, -2.0251952308; H, 2.2135401735, -0.4381131474, -2.2207906519; N, 1.4598282131, 1.6907838598, 0.2664036132; C, 1.9296514771, 2.9107556536, -0.4217320573; C, 1.3569715995, 1.8472851338, 1.7350840397; H, 0.5233923109, 1.4375660626, -0.0871696809; H, 2.9447140746, 3.147820328, -0.0972422681; H, 1.2797375466, 3.7610619455, -0.1988242076; H, 1.9301019445, 2.7393131827, -1.4984674496; H, 0.6826599785, 2.667402224, 1.9930939553; H, 2.3456914734, 2.0529003751, 2.1494224383; H, 0.9726462335, 0.9201658507, 2.1593197968.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4348334 (hartree), -

1958827.67709194 (kJ mol^{-1}).

TS23b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.950372 (hartree), -2479781.03288759 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.8811664061, -1.3070889924, 0.0484273158; C, 2.1677562384, -0.0981256874, 0.1448734559; C, 2.9708492952, 1.0559426539, 0.1067642968; C, 4.3471106343, 1.0350846816, -0.0173920477; C, 4.9983957189, -0.1947280285, -0.1093845129; C, 4.2577956216, -1.3747719048, -0.0756601687; N, 0.8054902293, 0.0387301835, 0.3042907494; C, -0.1085898313, -0.8263119454, 0.1182020525; C, -1.1622751862, -1.4614946517, -0.0521372551; C, -2.5216921392, -1.5953047625, -0.2658331586; N, -3.2638383279, -0.3402179361, 0.2632439638; C, -3.4145593054, -0.4344153515, 1.7356797819; O, -3.1999462195, -2.4668477482, -0.7752654693; C, -4.57724836, -0.1795512218, -0.3932145519; N, -1.6564925014, 1.6902708378, -0.2089133945; C, -1.586008094, 1.9092311223, -1.670889685; C, -2.0265472837, 2.9057689153, 0.5443561963; F, 2.3443693509, 2.2598763125, 0.1896641053; H, 4.8886187394, 1.9723036642, -0.0416517293; H, 6.0760026813, -0.2325693415, -0.2065552838; H, 4.7290859272, -2.3474719346, -0.1415499755; F, 2.1758868977, -2.4603401796, 0.0934144832; H, -2.4551443218, 0.7198932097, 0.021094315; H, -5.0472528393, 0.7360150961, -0.0251491304; H, -5.2262792664, -1.0330636013, -0.1886825069; H, -4.4397774976, -0.1102516892, -1.4721738827; H, -4.0195581859, -1.3052146151, 2.0060708374; H, -3.9050108262, 0.4672126715, 2.1119332513; H, -2.430028523, -0.5296156272, 2.1924871851; H, -0.7246419372, 1.3704424599, 0.1007679419; H, -3.0314060543, 3.2241407559, 0.2593523506; H, -1.3262511791, 3.7205299748, 0.3419512665; H, -2.0113364328, 2.6869279051, 1.6125099678; H, -0.8686051565, 2.6970703741, -1.9135328057; H, -2.5709042184, 2.194333536, -2.0460222818; H, -1.2732854769, 0.9813833925, -2.1495326072.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version =

AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9662188 (hartree), -2479822.61876896 (kJ mol^{-1}).

TS23c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4655751 (hartree), -2000896.26650013 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.0592115225, -1.2959006405, -0.047142907; C, 2.4702903765, -0.0397618413, 0.210253522; N, 3.1998665134, 1.0836570577, 0.3034167033; C, 4.5220599981, 0.986925236, 0.1440273066; C, 5.1949430644, -0.2038658426, -0.1117578687; C, 4.4322864774, -1.3699264563, -0.2083468078; N, 1.1032704818, 0.1216482934, 0.3946347589; C, 0.2151124217, -0.7625502283, 0.2011883689; C, -0.7962787156, -1.4653820758, 0.0175031118; C, -2.1453582966, -1.6300538455, -0.2407636302; N, -2.9329377623, -0.3837739753, 0.243895444; C, -3.1350408875, -0.4620381117, 1.7113408231; O, -2.7873869532, -2.5257116967, -0.7552876451; C, -4.225295672, -0.263059482, -0.4618875799; N, -1.3797293314, 1.6973415648, -0.1929433664; C, -1.2794157637, 1.9218439772, -1.6519895132; C, -1.8112001933, 2.8977815778, 0.5513066756; H, 5.0749979754, 1.9195950218, 0.2270116233; H, 6.2715888965, -0.2164441237, -0.2286780789; H, 4.9059204265, -2.325717614, -0.4064021063; H, 2.4345374953, -2.1789028146, -0.1139177974; H, -2.153207948, 0.6916901577, 0.0188047973; H, -4.7306911883, 0.644547815, -0.1222700812; H, -4.8596972527, -1.1303537938, -0.2704953125; H, -4.0499059498, -0.2021411918, -1.5358297206; H, -3.7251906278, -1.3457310962, 1.9720039895; H, -3.6636448802, 0.4305781849, 2.055717414; H, -2.1655776604, -0.5221284762, 2.2046204595; H, -0.443952912, 1.4119004961, 0.1402871239; H, -2.8208021965, 3.1796166346, 0.2448763514; H, -1.1375944331, 3.7384768237, 0.3641480821; H, -1.8104456741, 2.6796958522, 1.6197320866; H, -0.5824337132, 2.7333792812, -1.8757608741; H, -2.2632779821, 2.1746783512, -2.0524338126; H, -0.9227020514, 1.0067698791, -2.1245267695.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4824147 (hartree), -2000940.45773167 (kJ mol^{-1}).

TS23d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.460357 (hartree), -2000882.57292871 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.0660082294, -1.2473546849, -0.1645221002; C, 2.5011655057, -0.0221145033, 0.220220359; C, 3.3823718548, 1.057074718, 0.4130459797; N, 4.700907424, 0.9856903681, 0.2477953108; C, 5.2218736599, -0.1908252594, -0.1215300127; C, 4.4426385077, -1.3267604287, -0.3356556206; N, 1.1378375283, 0.1931700423, 0.4258140035; C, 0.2363577755, -0.6811159569, 0.2391438641; C, -0.7720092074, -1.3890867317, 0.06283368; C, -2.1088971887, -1.6303427209, -0.1939014061; N, -2.9590326933, -0.4183162122, 0.2568517307; C, -3.165585043, -0.4702415386, 1.7243707407; O, -2.6978161164, -2.5721599577, -0.6918772271; C, -4.2515814952, -0.3811751229, -0.4572299091; N, -1.4676215304, 1.696815208, -0.2360788556; C, -1.3720463865, 1.8765781135, -1.7028163643; C, -1.9413664341, 2.9041821411, 0.472377148; H, 2.9738058025, 2.0169397396, 0.7193511629; H, 6.2997922948, -0.2237942111, -0.2483093874; H, 4.9095736404, -2.259696702, -0.6316500006; H, 2.4291350426, -2.1113188798, -0.3214988048; H, -2.201044298, 0.6997857971, 0.000098144; H, -4.8035350062, 0.5094752624, -0.1458667252; H, -4.8449212511, -1.2727147334, -0.2451433354; H, -4.0741294538, -0.3422277131, -1.5319519925; H, -3.7144937906, -1.3743210652, 2.0055580891; H, -3.7380744677, 0.4040983514, 2.0451647582; H, -2.1974008557, -0.4729736595, 2.2241255438; H, -0.5291810561, 1.445700643, 0.1094845181; H, -2.9591682234, 3.1396667682, 0.1556075774; H, -1.2975122622, 3.7614708799, 0.259220782; H, -1.936035005, 2.7170663576, 1.5464733882; H, -0.702915498, 2.7037321168, -1.9515628078; H, -2.363652909, 2.084035409, -2.1091129355; H, -0.9859275406, 0.9579313064, -2.1436636343.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4784921 (hartree), -2000930.16386929 (kJ mol^{-1}).

TS23e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.463059 (hartree), -2000889.66363797 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.0570241755, -1.2164990645, -0.1797920988; C, 2.4973610187, 0.0083539309, 0.223863014; C, 3.3867834849, 1.0755960976, 0.4233857474; C, 4.7450051417, 0.8762353863, 0.2125443865; N, 5.2852844082, -0.2860379229, -0.1753109665; C, 4.4316524769, -1.3017408822, -0.3603515719; N, 1.1375008565, 0.2155403479, 0.4351861618; C, 0.2412900373, -0.6677252797, 0.2481294179; C, -0.7628259466, -1.37949078, 0.0743332241; C, -2.1002228368, -1.6295700116, -0.1798849506; N, -2.9571861389, -0.4262008128, 0.2752323463; C, -3.1438830676, -0.4697272224, 1.7461656629; O, -2.6808160004, -2.5727398375, -0.6821492174; C, -4.2591444775, -0.4048603751, -0.4227878955; N, -1.4884005383, 1.6962331897, -0.2463132775; C, -1.3918393478, 1.8565156515, -1.7153612073; C, -1.9748681146, 2.9090636189, 0.4439016053; H, 3.0090957476, 2.0396623808, 0.7439502349; H, 5.4411040719, 1.6972917311, 0.3650775219; H, 4.8749529111, -2.2438410254, -0.6729499108; H, 2.4244213514, -2.0809627502, -0.3464073037; H, -2.2152732602, 0.6921771797, 0.0036078748; H, -4.8136977638, 0.4838484294, -0.1109188409; H, -4.8427287791, -1.2991234732, -0.1959452574; H, -4.095673842, -0.3731537546, -1.4998484257; H, -3.6831922537, -1.3754038654, 2.0400460598; H, -3.7179704473, 0.4029924933, 2.0680450749; H, -2.1693558958, -0.4628704607, 2.2332337207; H, -0.5488300491, 1.458540354, 0.1047458219; H, -2.9947989156, 3.1293024969, 0.1230710136; H, -1.3401353526, 3.7700377783, 0.2182682354; H, -1.9685125364, 2.7382726541, 1.5207396568; H, -0.7306993737, 2.6868867418, -1.9746717203; H, -2.3847522376, 2.0486196969, -2.1260037256; H, -0.9958107482,

0.9359920605, -2.1432781434.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4816932 (hartree), -2000938.5643391 (kJ mol^{-1}).

TS14a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4237851 (hartree), -1958798.6836489 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, 1.2844692049, -0.5397289224, -0.0036370931; C, 0.2959196892, 0.1951303395, 0.0001601269; C, -0.3394053913, 1.3472591586, 0.0046545459; C, -1.304548781, 2.1625025779, 0.0086541487; O, -2.1798505511, 2.9576007201, 0.0124679967; C, 2.6411556207, -0.1754378899, -0.0047332162; C, 3.5912323817, -1.2051880691, -0.0094051382; C, 4.9498293334, -0.9065877266, -0.0107086839; C, 5.3783068163, 0.4208209231, -0.0073712833; C, 4.4340542178, 1.4479888875, -0.0027142245; C, 3.0728081962, 1.1601268275, -0.0013767505; N, -1.2508798759, -1.2873998632, -0.0017565178; C, -1.1039806319, -2.069571497, -1.2247794869; C, -1.1004157999, -2.0763284604, 1.2164822486; H, 3.2457644291, -2.2322347223, -0.0119645617; H, 5.6756134423, -1.7122242879, -0.0143384949; H, 6.4370688192, 0.6530175376, -0.0083876086; H, 4.7590945659, 2.4826751343, -0.0000983977; H, 2.34096504, 1.9587750226, 0.0022388427; H, -2.1357044721, -0.7639730582, 0.000966439; H, -1.7846498539, -2.9317536435, -1.2512410572; H, -0.0752997278, -2.4334836617, -1.2907652752; H, -1.3038045448, -1.4358058623, -2.0905248619; H, -0.0715613069, -2.4406253859, 1.2774177344; H, -1.7810427028, -2.9386238367, 1.2401793904; H, -1.2976660444, -1.4473557435, 2.0863038048; N, -4.0510643319, 0.2049459889, 0.0068088859; C, -4.8121242876, -0.0812903696, -1.2109600168; C, -4.8083521084, -0.0887216213, 1.2251599921; H, -3.7911049093, 1.1874534959, 0.0093906936; H, -5.7887227067, 0.4270918913, -1.2428372148; H, -4.9938342575, -1.1576553772, -1.2867022795; H, -4.2363317912,

0.2269144634, -2.0862439799; H, -4.9898074397, -1.1655343283, 1.2949152115; H, -5.7848570159, 0.4194211953, 1.2631469649; H, -4.2298656261, 0.2141765017, 2.1005201796.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4305825 (hartree), -1958816.52169002 (kJ mol^{-1}).

TS14b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9513819 (hartree), -2479783.68311234 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.802484156, 1.156167677, 0.447640768; C, 2.3102142259, -0.0840636871, 0.0103266533; C, 3.2840137423, -1.0182054003, -0.3751163816; C, 4.6407145035, -0.7484495491, -0.3614757737; C, 5.074814821, 0.5033601052, 0.0707737656; C, 4.1521369761, 1.4618239589, 0.4835239995; N, 0.9743112066, -0.4482535971, 0.0069401193; C, -0.0395408452, 0.2162973901, -0.2284793802; C, -0.7251808027, 1.2515193942, -0.6448602009; C, -1.7129065037, 1.9854576201, -0.9297395078; O, -2.6143309862, 2.69582574, -1.2090248571; N, -1.5138908695, -1.2642684368, 0.2225911972; C, -1.2478081939, -1.7910455437, 1.5564627167; C, -1.430739862, -2.2742001959, -0.8304351388; N, -4.3419767706, 0.1570808244, 0.1513738409; C, -4.8068632915, 0.47854899, 1.5025298627; C, -5.3181479698, -0.6260520276, -0.6085995998; F, 2.864032841, -2.2325780446, -0.7910002374; H, 5.3334427441, -1.5140281348, -0.6864502827; H, 6.1333042166, 0.7306691911, 0.089043802; H, 4.4591999765, 2.438633256, 0.8348896026; F, 1.9140589342, 2.0739558593, 0.8811138972; H, -2.4136564658, -0.7675172344, 0.1897199319; H, -2.1111185477, -3.1172241371, -0.6482861919; H, -0.407699982, -2.6547416377, -0.8800037401; H, -1.681166104, -1.8210051363, -1.791241215; H, -0.2000368195, -2.0981175927, 1.611981395; H, -1.8810598133, -2.656711497, 1.7944160067; H, -1.421162459, -1.0109983943, 2.2997902982; H, -4.1544503066, 1.0239922627, -0.3447965587; H, -6.3113633029, -

0.1525819435, -0.6595681358; H, -5.4411385738, -1.6094276061, -0.1448679025; H, -4.9568057895, -0.7766166323, -1.6281562601; H, -4.9015003117, -0.4414137693, 2.0873244271; H, -5.7836324502, 0.9872384509, 1.5166838758; H, -4.0775848001, 1.1219803761, 1.9990500665.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9591021 (hartree), -2479803.9428065 (kJ mol^{-1}).

TS14c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4675943 (hartree), -2000901.56537509 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1082747536, 1.154839537, -0.0008377; C, -2.659125861, -0.1774041407, -0.0008054818; N, -3.4924230278, -1.2231063318, -0.0013018763; C, -4.8035076129, -0.9744647207, -0.0018522293; C, -5.3513614208, 0.3060085575, -0.001936805; C, -4.4752030144, 1.3905278191, -0.0014132226; N, -1.2989131727, -0.4981812094, -0.0002479139; C, -0.319225714, 0.2438672928, 0.0002043761; C, 0.3247507991, 1.3884196158, 0.0005526924; C, 1.3048029044, 2.1878982016, 0.0008998208; O, 2.1889006008, 2.9704324986, 0.0011733673; N, 1.2369795994, -1.2701663434, 0.000821932; C, 1.0639059598, -2.0529558845, -1.2183884584; C, 1.0639069934, -2.0517957361, 1.2207863865; N, 4.0617124688, 0.1939315586, 0.0004632331; C, 4.8145126596, -0.1111708166, -1.2177207741; C, 4.8146755408, -0.1114047679, 1.2184889735; H, -5.4496741539, -1.8481708981, -0.0022469642; H, -6.4255454531, 0.4448313184, -0.002395296; H, -4.8517646022, 2.4075421693, -0.0014532674; H, -2.3933174326, 1.9680592528, -0.0004219865; H, 2.1327735315, -0.7675419907, 0.0005982632; H, 1.7208683466, -2.9324121546, 1.2473472625; H, 0.0256054342, -2.3892253326, 1.2799274436; H, 1.2777450573, -1.4270655977, 2.0900369345; H, 0.0255283478, -2.3901918451, -1.2773385574; H, 1.7206714938, -2.9337477788, -1.2439893133; H, 1.2779992146, -1.4291302436, -2.0882248674; H, 3.8196537722,

1.1808200916, 0.0005845222; H, 5.8010660609, 0.3775926416, 1.2544034046; H, 4.9749474906, -1.1913801656, 1.2901550511; H, 4.243108174, 0.2039640795, 2.0939938536; H, 4.9747855045, -1.1911312145, -1.2896079674; H, 5.8008935886, 0.3778423926, -1.2536796377; H, 4.2428208623, 0.204351825, -2.0930889099.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4759359 (hartree), -2000923.45577492 (kJ mol^{-1}).

TS14d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4638495 (hartree), -2000891.73810342 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.1221037548, 1.17192719, -0.0294689356; C, -2.6562471892, -0.1479013748, 0.0197241167; C, -3.6059805433, -1.1794757071, 0.0650542173; N, -4.9209315355, -0.9741227543, 0.0639046546; C, -5.3536198058, 0.2909325125, 0.0166803717; C, -4.4947591573, 1.387966029, -0.0307327529; N, -1.3015953304, -0.5020750256, 0.0264890306; C, -0.3225864654, 0.2426819101, -0.0078333184; C, 0.3286339711, 1.3785691438, -0.0557472961; C, 1.3011143439, 2.1867708045, -0.0926065376; O, 2.1802713898, 2.9729078929, -0.1280356993; N, 1.2569691693, -1.2889476518, 0.0438981564; C, 1.0929910126, -2.1189768534, -1.1439364405; C, 1.1054703704, -2.0238155006, 1.2944168675; N, 4.0685470301, 0.2017027356, -0.0289508944; C, 4.8160260958, -0.1490708553, -1.2383822521; C, 4.8291420117, -0.054098441, 1.1960184543; H, -3.2630111631, -2.2095620915, 0.1035566013; H, -6.4304131662, 0.4309873955, 0.0168392125; H, -4.896266619, 2.3941415859, -0.0679922799; H, -2.4211995963, 1.9975805763, -0.0654394751; H, 2.1454714688, -0.77423216, 0.0192581371; H, 1.7753160495, -2.8935336764, 1.3528909475; H, 0.0733851818, -2.3749924278, 1.3786362278; H, 1.3152591606, -1.3619628464, 2.136680732; H, 0.06025282, -2.4752813729, -1.1899563017; H, 1.762584971, -

2.9908479105, -1.141319073; H, 1.2938532427, -1.5248492331, -2.0373207207; H, 3.8256806146, 1.1876496138, -0.0661282014; H, 5.8144601917, 0.4380085539, 1.2069990105; H, 4.9924292781, -1.130066778, 1.308924765; H, 4.2618288277, 0.2941690722, 2.0617689093; H, 4.978511851, -1.2306373271, -1.2688893279; H, 5.8009756373, 0.3402455716, -1.2982524348; H, 4.2392994579, 0.1309660371, -2.1224767305.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4720296 (hartree), -2000913.20468773 (kJ mol^{-1}).

TS14e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4650302 (hartree), -2000894.83654918 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.1087128611, 1.1509784949, -0.0002636726; C, 2.6492142494, -0.1733459095, -0.0001000618; C, 3.6048155895, -1.1951715055, -0.0000326716; C, 4.9522889262, -0.8527767049, -0.000129415; N, 5.4038432514, 0.4064854349, -0.0002841466; C, 4.4813298511, 1.3755743131, -0.0003478639; N, 1.2947463842, -0.5249613199, -0.0000009621; C, 0.3175767247, 0.2263810705, -0.0000506876; C, -0.3262360588, 1.3657326698, -0.0001623519; C, -1.2916027018, 2.1839518872, -0.0002246563; O, -2.163044358, 2.9780932236, -0.0002849476; N, -1.2631495107, -1.291388376, 0.000184446; C, -1.1095699969, -2.0751333064, 1.2205599896; C, -1.1096865646, -2.075364692, -1.2200568856; N, -4.0650774169, 0.2076264125, 0.0001947254; C, -4.8191523949, -0.0961637536, 1.2185143367; C, -4.819330987, -0.09650417, -1.2179292081; H, 3.290206405, -2.2315148951, 0.0000926703; H, 5.7092612454, -1.6321675188, -0.0000794063; H, 4.8599077049, 2.3940660119, -0.0004740153; H, 2.4125231526, 1.9803517465, -0.0003224566; H, -2.1489899066, -0.7708371436, 0.0001792298; H, -1.7832691453, -2.9435427974, -1.2466855788; H, -0.0787116635, -2.4336861296, -1.2855884005; H, -1.3130990596,

-1.4461929191, -2.0884590748; H, -0.0785868954, -2.4334359797, 1.2860658905; H, -1.7831453115, -2.9433100297, 1.2474130493; H, -1.3129083989, -1.4457986307, 2.0888614647; H, -3.8241132988, 1.1947351632, 0.0000391937; H, -5.8047465192, 0.3940291901, -1.2529410511; H, -4.9814271973, -1.1761718264, -1.289384517; H, -4.2478743287, 0.2181450968, -2.0937551531; H, -4.9812315556, -1.1758120879, 1.2903003165; H, -5.8045657297, 0.3943736904, 1.2535299988; H, -4.2475705794, 0.2187378483, 2.0941678699.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4734662 (hartree), -2000916.97467771 (kJ mol^{-1}).

Int4a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4334858 (hartree), -1958824.14065975 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.4645856861, -0.1852342072, -1.698014862; C, 2.4633539011, -0.2138490557, -0.2903273073; C, 3.6971724674, -0.337565446, 0.3757289482; C, 4.889250118, -0.4295374748, -0.331320186; C, 4.8804866282, -0.4002756183, -1.7269491813; C, 3.664814315, -0.278064638, -2.3985296791; N, 1.3343906582, -0.129868461, 0.5319834318; C, 0.1252554055, -0.0135530578, 0.1189995886; N, -0.8380302357, 0.0470584125, 1.363933311; C, -0.5484641109, 1.2419799957, 2.2030919039; C, -0.5387843098, 0.0700706543, -1.0769912029; C, -1.6105660108, 0.1790117759, -1.7293246724; O, -2.5955765143, 0.2804813843, -2.3978605784; C, -0.7676961336, -1.2132318696, 2.1529822329; N, -3.7112694588, 0.3184581635, 0.6201633013; C, -4.2992836746, 1.5861375454, 1.069673085; C, -4.5156576084, -0.8425218513, 1.0200611146; H, 3.6918257963, -0.3592059248, 1.4596589469; H, 5.827130226, -0.524201235, 0.2053980229; H, 5.8087298758, -0.4717874238, -2.2826506626; H, 3.6470889748, -0.2543508351, -3.4830743888; H, 1.5275441196, -0.0907509919, -2.2295820651; H, -1.8188804072,

0.1420364942, 1.0013011111; H, -1.4728797174, -1.156990513, 2.9838193582; H, 0.250688008, -1.3361050138, 2.5144041898; H, -1.0279928614, -2.0451378797, 1.4998012009; H, 0.4742733224, 1.1678200274, 2.5655009892; H, -1.2554473326, 1.2779280987, 3.0335237152; H, -0.6549544202, 2.132585639, 1.5850718368; H, -3.6543492232, 0.3341786029, -0.3971658408; H, -5.5625805588, -0.7699695759, 0.6913157649; H, -4.5129698231, -0.9382126536, 2.1099989168; H, -4.0858954209, -1.7514749301, 0.5943337119; H, -4.2836924144, 1.6355954007, 2.1625762121; H, -5.3413489585, 1.7131181726, 0.7420125561; H, -3.7141138564, 2.4213361458, 0.6796020495.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.445683 (hartree), -1958856.14909756 (kJ mol^{-1}).

Int4b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9645095 (hartree), -2479818.13314745 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.7503080587, -1.5593204129, 0.6031281901; C, 2.4881735162, -1.0121027888, 0.7602265572; C, 2.1133740239, 0.2270974797, 0.2242561054; C, 3.1172704445, 0.8977732259, -0.4844159819; C, 4.3908713579, 0.3885443392, -0.6723025158; C, 4.7060938045, -0.8527988851, -0.1235347154; N, 0.875464605, 0.8262759593, 0.4559934159; C, -0.1934410482, 0.2937788138, -0.0232961194; C, -0.4746814309, -0.7644461883, -0.8417702868; C, -1.3363492721, -1.4514382105, -1.4539006651; O, -2.1070488142, -2.1390554757, -2.0503887596; N, -1.4341095263, 1.1262419793, 0.4093069504; C, -1.4547831488, 1.3878091516, 1.87599596; C, -1.4966374946, 2.3898170521, -0.3813500669; N, -3.9319908716, -0.3355170864, -0.0928636827; C, -4.1984842867, -1.2518859997, 1.0253725715; C, -5.0968642994, 0.4927223068, -0.4273615978; F, 2.8124693495, 2.1049840639, -1.0207561988; H, 5.1101403768, 0.9612585908, -1.2438490824; H, 5.6964273299, -1.2687144935, -0.2613028897; H, 3.9662462218, -

2.5226887014, 1.0473986756; F, 1.5753636909, -1.6855542402, 1.4997955497; H, -2.2916413144, 0.5574537679, 0.1767276823; H, -2.3720664888, 1.9243760991, 2.1235257704; H, -0.5765175442, 1.9708863518, 2.1405232251; H, -1.4267110426, 0.4328421545, 2.3983952365; H, -0.6111594559, 2.9813174797, -0.1574824364; H, -2.4040954916, 2.9344635601, -0.1168940642; H, -1.5105092519, 2.1325885182, -1.4394603608; H, -3.6851173626, -0.8991024351, -0.9049861778; H, -5.0782516375, -1.8871789363, 0.8516352196; H, -4.3729653271, -0.6774488877, 1.9398699242; H, -3.3327640099, -1.8977742914, 1.1815503097; H, -5.3218890116, 1.1677219444, 0.4036322505; H, -5.9989053969, -0.1021740669, -0.6306451317; H, -4.8789782424, 1.0974434683, -1.3102236276.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9784627 (hartree), -2479854.749759 (kJ mol^{-1}).

Int4c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4778964 (hartree), -2000928.60060671 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.1230515503, 1.4877929812, -0.0000581825; C, -2.7909487417, 1.096955525, -0.0000355306; C, -2.484797068, -0.2790035566, -0.0000258698; N, -3.4519654648, -1.2177163758, -0.0000380124; C, -4.7223826884, -0.8191884478, -0.000060115; C, -5.1211648025, 0.5166123311, -0.0000711237; N, -1.1979198859, -0.8090850539, -0.0000024516; C, -0.1091304809, -0.1301622472, 0.000003408; C, 0.2735283427, 1.184519444, -0.000008106; C, 1.180565196, 2.0599545267, -0.0000075363; O, 1.9936166785, 2.9331299027, -0.0000079916; N, 1.105220069, -1.132625578, 0.0000325251; C, 1.0964420007, -1.9695367347, 1.2322907674; C, 1.0964647727, -1.9695835483, -1.2321939876; N, 3.7590622737, 0.2256310098, 0.0000348737; C, 4.5316887981, -0.0411299548, 1.219561023; C, 4.5317021308, -0.041151079, -1.2194782552; H, -5.4667330019, -1.6120328522, -0.00006953; H, -6.1723129847,

0.7792018657, -0.0000890998; H, -4.3771602789, 2.5425271073, -0.0000658759; H, -1.9918284153, 1.8253500316, -0.0000255898; H, 1.9896465479, -0.5672135453, 0.0000305655; H, 1.9608583484, -2.6351257867, 1.2190515075; H, 0.1675226706, -2.5352067204, 1.2540858618; H, 1.1472496174, -1.3110902296, 2.098604575; H, 0.1675428388, -2.5352492609, -1.2539878786; H, 1.9608774686, -2.6351765079, -1.2189103759; H, 1.1472949246, -1.3111704033, -2.0985318104; H, 3.4887093688, 1.2078578006, 0.0000250915; H, 5.4870254619, 0.5028043681, 1.2469644569; H, 4.7528025079, -1.1101448372, 1.2918277008; H, 3.9477092912, 0.2485734734, 2.0954389482; H, 4.7528166441, -1.1101672058, -1.2917238968; H, 5.4870390197, 0.5027828855, -1.2468806569; H, 3.9477321443, 0.2485371431, -2.0953675535.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4921614 (hartree), -2000966.03545777 (kJ mol^{-1}).

Int4d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4755816 (hartree), -2000922.52600501 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.2023130282, 0.0001320178, -4.3907431696; C, -0.2480307897, 0.0000868396, -3.0000549322; C, 0.9630723557, 0.0001100457, -2.2878393561; C, 2.1501328889, 0.0001780961, -3.0482496656; N, 2.1974171076, 0.0002205736, -4.3765380697; C, 1.031097108, 0.0001973876, -5.0360593955; N, 1.1281088198, 0.0000728319, -0.903334911; C, 0.1646310521, 0.0000067724, -0.0530968757; C, -1.2049499403, -0.0000479593, -0.0821869937; C, -2.309533108, -0.0001144799, 0.525329322; O, -3.3839395256, -0.0001759021, 1.0443851405; N, 0.7600804668, -0.0000171642, 1.3989726246; C, 1.5575178726, -1.2332122339, 1.6481603116; C, 1.5574360104, 1.2332152058, 1.6482370433; N, -1.3175110832, -0.0001525575, 3.523775719; C, -1.2920899135, -1.2198165727, 4.341221999; C, -1.2921816075,

1.2194699642, 4.3412867216; H, 3.0997903418, 0.000197349, -2.5193675435; H, 1.0911326081, 0.0002330941, -6.1205517817; H, -1.1187465673, 0.0001160393, -4.9704874674; H, -1.1907010578, 0.0000356376, -2.4695308121; H, -0.0456325021, -0.0000653681, 2.074187504; H, 1.9209380896, -1.2227425973, 2.6768391318; H, 2.3854714965, -1.2565117333, 0.943448616; H, 0.9152903428, -2.0984836347, 1.4893021388; H, 2.3853858415, 1.2566152779, 0.9435242306; H, 1.9208599791, 1.2227036872, 2.6769141296; H, 0.9151503283, 2.0984539106, 1.489436381; H, -2.1764191565, -0.0001708123, 2.9756883555; H, -2.0952597434, -1.2466649108, 5.0916239748; H, -0.3371267507, -1.2918942978, 4.8701241394; H, -1.3956413996, -2.0958211379, 3.6978080769; H, -0.3372240356, 1.2915911415, 4.8701929935; H, -2.0953536475, 1.2462182464, 5.0916898895; H, -1.3957985424, 2.0955010393, 3.6979193254.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4897023 (hartree), -2000959.58217755 (kJ mol^{-1}).

Int4e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4764004 (hartree), -2000924.67473659 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.1644630516, 0.000131715, -4.3824815083; C, -0.2113809045, 0.0000855371, -2.9911023968; C, 0.9979773549, 0.0001065394, -2.2731360281; C, 2.1811829116, 0.0001738663, -3.0327426453; C, 2.1090487485, 0.0002155824, -4.4184100171; N, 0.9598416496, 0.0001957899, -5.106866386; N, 1.147440632, 0.0000675952, -0.8873501918; C, 0.1715671358, 0.0000053197, -0.0476949811; C, -1.194615105, -0.0000428883, -0.0867281362; C, -2.3070947893, -0.0001020745, 0.5071555364; O, -3.3868059116, -0.0001571213, 1.0122618407; N, 0.7539154778, -0.0000209356, 1.4105253858; C, 1.5490045986, -1.2333860545, 1.6667361671; C, 1.5489273602, 1.2333780341, 1.6668124793; N, -1.3404179235, -

0.000152587, 3.5167233202; C, -1.3199467686, -1.2199226921, 4.3345265153; C, -1.3200339916, 1.2195771891, 4.3345888265; H, 3.1385143185, 0.0001923556, -2.5249766667; H, 3.0206717597, 0.0002676829, -5.0103124963; H, -1.0928844935, 0.0001160277, -4.9478264978; H, -1.1612167378, 0.0000344915, -2.4752939918; H, -0.0580554718, -0.0000674654, 2.078670242; H, 1.9029808083, -1.2225968877, 2.6986449509; H, 2.3831588131, -1.2567046632, 0.9694249181; H, 0.9082091005, -2.0987024849, 1.5023563075; H, 2.3830772803, 1.2567943888, 0.9694994011; H, 1.9029082427, 1.2225448672, 2.6987192299; H, 0.9080764194, 2.098664479, 1.502490924; H, -2.1964090805, -0.0001694509, 2.9642634383; H, -2.1276828579, -1.246623377, 5.0798918554; H, -0.3682675282, -1.2916917697, 4.8692871735; H, -1.4194256645, -2.0960445894, 3.6906414442; H, -0.3683598131, 1.2913870206, 4.8693530114; H, -2.1277718787, 1.2461819793, 5.0799556756; H, -1.4195757698, 2.0957248854, 3.6907485881.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4909603 (hartree), -2000962.88347742 (kJ mol^{-1}).

TS24a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4221927 (hartree), -1958794.5048016 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, 0.6952218136, -1.1490401353, 0.1009452951; C, -0.3487101147, -0.4901254579, -0.2676674632; C, -0.5750693381, 0.8170325921, -0.73113465; C, 0.0558833367, 1.8536786353, -1.1309278075; O, 0.4981210348, 2.8810987051, -1.5146151644; C, 1.9678960483, -0.5702426791, 0.1953900331; C, 3.0490360415, -1.2404362311, -0.3982275199; C, 4.3447705363, -0.748204136, -0.2764099763; C, 4.5945441234, 0.4099796132, 0.459630648; C, 3.5290193983, 1.0712548693, 1.0695104162; C, 2.2284998237, 0.5931851221, 0.937625887; N, -1.6181017931, -1.2955918816, -0.1965010407; C, -2.020347413, -

1.724866804, -1.5567184976; C, -1.5525368498, -2.4507646638, 0.7196814328; H, 2.8518200699, -2.1496792136, -0.954737688; H, 5.1642406708, -1.2759969103, -0.7527736349; H, 5.6049255307, 0.7897768306, 0.5594984361; H, 3.7096593086, 1.9704840782, 1.6488491696; H, 1.4080535631, 1.1160949247, 1.4137050195; H, -2.5550088028, -0.3483926167, 0.2274805132; H, -3.0135351794, -2.1799236153, -1.519941467; H, -1.3072498744, -2.4551398996, -1.9526560903; H, -2.0364427513, -0.8541181647, -2.2117451742; H, -0.8271024617, -3.190937012, 0.3778567365; H, -2.5462236103, -2.9043469862, 0.7750476171; H, -1.2472252462, -2.1149806428, 1.7100484326; N, -3.1564844159, 0.6914734996, 0.4753622868; C, -4.4581326274, 0.8084846312, -0.2045795681; C, -3.1915245666, 0.9838009129, 1.9200858554; H, -2.4311066226, 1.2776876032, 0.0064593734; H, -4.8886232513, 1.8027033945, -0.0568976992; H, -5.1508494263, 0.0616044568, 0.1890331566; H, -4.3191712384, 0.6398487373, -1.2726286667; H, -3.8247283133, 0.2549929737, 2.4300539168; H, -3.5825160729, 1.9876281479, 2.1064965898; H, -2.1783041943, 0.9193554691, 2.317574247.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -746.4377455 (hartree), -1958835.31915502 (kJ mol^{-1}).

TS24b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9584381 (hartree), -2479802.200308 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.8381333561, -1.0161525564, -0.8219160883; C, 1.6241218847, 0.3164151446, -0.4445248024; C, 2.7689990224, 0.995514038, -0.007982922; C, 4.0237750093, 0.4135805542, 0.0606564085; C, 4.1733200747, -0.9166908455, -0.3248736709; C, 3.0712655376, -1.6411565204, -0.7747443774; N, 0.4019380244, 0.9626129046, -0.5996586461; C, -0.5878757286, 0.6730164641, 0.1819089364; N, -1.8743398858, 1.3188952367, -0.2236013461; C, -1.8421415402, 1.9975343338, -1.5353055631; C, -0.7263047069, -

0.163253226, 1.2911292977; C, -0.0261278331, -0.8386629244, 2.1185330242; O, 0.4888801514, -1.5021720803, 2.950452042; C, -2.382672162, 2.2253212471, 0.8346859468; N, -3.1928517028, -0.9146943118, -0.1102934263; C, -2.8838444735, -1.7886718824, -1.2615006227; C, -4.614471038, -0.8933162849, 0.2758931308; F, 2.6308387786, 2.2890879946, 0.3685161687; H, 4.8590693031, 1.002344269, 0.4181288406; H, 5.1463830434, -1.388976946, -0.273813244; H, 3.1537309396, -2.6755016386, -1.0836514759; F, 0.7695784188, -1.7215662485, -1.2881333053; H, -2.6736330169, 0.2261923805, -0.2557139722; H, -3.4002689097, 2.5362850185, 0.5870738804; H, -1.7460645158, 3.1118529689, 0.9127484315; H, -2.3719708973, 1.6946327927, 1.7854073361; H, -1.161202744, 2.8503701847, -1.5226164143; H, -2.8545541233, 2.3368578235, -1.7691648111; H, -1.4966472917, 1.3037816215, -2.2990318135; H, -2.5933978667, -1.1803445433, 0.6875268384; H, -4.9790520847, -1.9007533904, 0.4957578617; H, -5.2095049478, -0.4742529266, -0.5381463787; H, -4.7374593717, -0.2712147455, 1.1630568431; H, -3.3918533476, -1.4122219212, -2.1515131823; H, -3.2122377262, -2.8143256483, -1.0720123406; H, -1.8064218975, -1.783606429, -1.427976762.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -944.9741521 (hartree), -2479843.43768967 (kJ mol^{-1}).

TS24c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4668587 (hartree), -2000899.63498066 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.2424386188, 0.5406652234, 1.0108425769; C, 1.9802723306, -0.5787767942, 0.1986697909; N, 2.9524294063, -1.2156534453, -0.469513295; C, 4.1996112046, -0.7493460505, -0.3604410119; C, 4.5581109102, 0.344537964, 0.4206570162; C, 3.5457941638, 0.998427168, 1.1231890138; N, 0.7105615598, -1.1498499265, 0.1176480164; C, -0.3307256817, -0.4869227424, -0.2479933631; N, -1.6003470264, -

1.2878836142, -0.1851582496; C, -1.5405349271, -2.4376077921, 0.7393573757; C, -0.5454054273, 0.8251227308, -0.7028891154; C, 0.0975839319, 1.8585724819, -1.0919538514; O, 0.5533075511, 2.8835698733, -1.4659049461; C, -1.9732566397, -1.7323366163, -1.5502545505; N, -3.1580619135, 0.7017688415, 0.439856214; C, -3.2489058735, 0.989580681, 1.8830350717; C, -4.4332099453, 0.8186597525, -0.2896017758; H, 4.9548266921, -1.2882407984, -0.92744407; H, 5.5898240137, 0.670061412, 0.4754469282; H, 3.7703084352, 1.8577036441, 1.7460830555; H, 1.4305316392, 1.0295173517, 1.5340640888; H, -2.5523669405, -0.3346826649, 0.2132625636; H, -2.9615572123, -2.1984321856, -1.5261319589; H, -1.243426392, -2.4555457373, -1.9272971738; H, -1.9887548234, -0.8671814407, -2.2127082843; H, -0.7961659734, -3.1679153766, 0.4178433482; H, -2.529003843, -2.9038690698, 0.7744694526; H, -1.264575101, -2.0919155308, 1.7352448806; H, -2.4172282474, 1.2899009996, -0.0011091989; H, -4.8710511618, 1.8113051289, -0.1541573486; H, -5.1384050655, 0.0683664346, 0.0739688187; H, -4.252235939, 0.6548466309, -1.352013982; H, -3.9018495814, 0.2595535385, 2.3654690758; H, -3.6460845532, 1.9930411964, 2.0572808609; H, -2.2519565299, 0.9227984551, 2.3194366488.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4854848 (hartree), -2000948.51442541 (kJ mol^{-1}).

TS24d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4639793 (hartree), -2000892.07873039 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.2520153861, 0.6331748401, -3.8128076738; C, -0.3002217687, 0.5784577231, -2.4240424218; C, 0.8775264409, 0.7922933614, -1.6942327736; C, 2.0429677029, 1.0662323848, -2.4351561864; N, 2.0980885873, 1.1065466217, -3.7645376733; C, 0.9634539139, 0.8909227293, -4.4409469137; N, 0.9677252953,

0.8496661049, -0.3031048359; C, 0.3919998226, 0.0079975483, 0.4879439572; C, -0.3624067636, -1.1593930286, 0.30087609; C, -0.7120514577, -2.0144531858, -0.5790903015; O, -1.1199660123, -2.8696065917, -1.2877056342; N, 0.5734944019, 0.3424355444, 1.9424955189; C, 1.591554761, -0.5531392616, 2.5425172456; C, 0.9023250972, 1.7576241497, 2.2040716143; N, -1.7586755595, -0.5136947452, 2.7214828929; C, -1.8064775374, -1.3104158804, 3.9608235093; C, -2.8522803718, 0.4664085559, 2.5813291429; H, 2.9671342222, 1.2575941725, -1.8964846226; H, 1.0314045475, 0.9328822326, -5.5241009244; H, -1.1474434872, 0.4733064218, -4.4029237798; H, -1.2342021865, 0.3838985156, -1.9127431429; H, -0.6636871406, -0.016418471, 2.4958839676; H, 1.6192421038, -0.4035462003, 3.624849321; H, 2.5812724576, -0.3383387852, 2.1269689683; H, 1.3302567668, -1.5871078333, 2.3188387798; H, 1.8721944547, 2.0271847226, 1.782818613; H, 0.9124611821, 1.9146679559, 3.2862591163; H, 0.1485397808, 2.3985989834, 1.7482010732; H, -1.7174847558, -1.127981589, 1.8821339828; H, -2.7617514938, -1.8341073665, 4.0521185807; H, -1.6773900224, -0.6566338552, 4.825745331; H, -1.0012057774, -2.0449377761, 3.9439610017; H, -2.7882098943, 1.2072204556, 3.3806232602; H, -3.8267961132, -0.0264562508, 2.6292087075; H, -2.7552823401, 0.9680931035, 1.6182237908.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4817597 (hartree), -2000938.73885137 (kJ mol^{-1}).

TS24e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.46629 (hartree), -2000898.14257269 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.244317699, 0.5886147239, 0.9271692138; C, 1.9697528422, -0.5664697955, 0.1774821025; C, 3.0693366115, -1.2183938065, -0.4010620862; C, 4.3435497291, -0.6943150993, -0.2221056627; N, 4.6111587326,

0.4044227172, 0.4938992398; C, 3.5609373656, 1.0167658682, 1.0528270022; N, 0.7063779698, -1.1399156852, 0.0663714956; C, -0.34337661, -0.4769819731, -0.2893246756; N, -1.6090229294, -1.2836321756, -0.2122343673; C, -1.5343728907, -2.4459371851, 0.6954144211; C, -0.5693856551, 0.8283020278, -0.7432818965; C, 0.0562680577, 1.8694338517, -1.1414465699; O, 0.4935749318, 2.8982602344, -1.5224610801; C, -2.0266573376, -1.7025832151, -1.5720733518; N, -3.1571417182, 0.6833108554, 0.4963114884; C, -3.1748213276, 0.9582750638, 1.9455084788; C, -4.4737517517, 0.7809364384, -0.1589865513; H, 2.9158096208, -2.1224625852, -0.9783140765; H, 5.19960028, -1.1892340365, -0.6738004011; H, 3.7836129388, 1.9070709912, 1.6354216879; H, 1.4455152866, 1.1376816855, 1.4093349689; H, -2.5373504072, -0.3495074622, 0.2262600961; H, -3.0173358071, -2.1615986402, -1.5257194195; H, -1.3158906209, -2.4267452338, -1.982428544; H, -2.0544206809, -0.8263931585, -2.219165743; H, -0.8141890061, -3.1842712348, 0.3392857729; H, -2.5277713605, -2.8984783642, 0.7583663509; H, -1.2181630115, -2.1175863666, 1.6847630884; H, -2.4584787405, 1.2933226759, 0.0255998486; H, -4.9221864442, 1.7641365636, 0.0074139025; H, -5.1428053382, 0.0156568086, 0.2397987066; H, -4.3517160079, 0.6258613944, -1.2311226272; H, -3.7849492265, 0.2102494738, 2.4554945789; H, -3.5836814225, 1.9512457527, 2.1504683923; H, -2.1545842842, 0.9097884818, 2.3268745176.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -762.4846254 (hartree), -2000946.25914949 (kJ mol^{-1}).

TS15a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8575268 (hartree), -2668483.00484888 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.6825315544, 5.0391660577, -0.3930213148; C, 2.2067836189, 3.7557524904, -0.2300923269; C, 1.3694471123,

2.6488980806, -0.1300294347; C, -0.0215120319, 2.8276337148, -0.1950529782; C, -0.5489205432, 4.1153729499, -0.3534728308; C, 0.3002154853, 5.2131267373, -0.4533516534; N, -0.9289775646, 1.7582166156, -0.1016984235; C, -0.706210781, 0.5457273897, -0.0423579587; C, -0.5913263237, -0.7105660839, 0.0170239641; C, -0.7456766803, -2.0101199646, 0.0733907968; N, -2.7565247572, -2.276852023, 0.2107017895; C, -3.027703089, -2.8908158509, 1.5124389337; O, -0.2965262921, -3.1130892664, 0.0860754466; C, -3.1722101938, -3.1093416293, -0.9195153856; N, -4.0764597147, 0.5366843889, 0.0422219181; C, -4.8668484566, 0.871129876, 1.2284573357; C, -4.8177637443, 0.7456118363, -1.2031215253; N, 2.9016173673, -2.8969102102, -0.7018211846; C, 2.8772976638, -2.6133205963, -2.1344473517; C, 3.7497742053, -4.0352386915, -0.3605429148; N, 3.5493241059, -0.095615652, 0.8119645404; C, 4.9594264089, 0.2396892382, 0.6718125425; C, 3.1328537403, -0.2116902027, 2.2031527971; H, -1.6248674683, 4.2373906272, -0.3987468616; H, -0.1189695658, 6.2055051993, -0.5780808808; H, 2.3446195057, 5.8941114858, -0.470323618; H, 3.280197305, 3.6096882012, -0.1790215774; H, 1.7990708938, 1.65972039, 0.005928808; H, -3.1819478757, -1.3381738065, 0.1523921139; H, -4.2296505927, -3.3939274639, -0.8490881137; H, -2.5640987927, -4.0167045891, -0.9381880841; H, -3.0135952808, -2.5633396855, -1.8507369694; H, -2.4242307304, -3.7957098741, 1.6144235113; H, -4.0860364696, -3.1581904028, 1.6243664856; H, -2.7522088288, -2.1950715359, 2.3064502428; H, -3.2406663128, 1.118005235, 0.0271606838; H, -5.2313234282, 1.762231668, -1.2962998585; H, -5.6525377298, 0.0401504518, -1.2599528802; H, -4.1613295449, 0.5643308554, -2.0568234395; H, -5.7075815984, 0.1765920378, 1.3203042699; H, -5.2776046074, 1.892822132, 1.2027106423; H, -4.2478999095, 0.7741640259, 2.1230306418; H, 3.3545072687, -0.9725031454, 0.3252873701; H, 3.7395039056, -0.9247915396, 2.7909952463; H, 3.2023393373, 0.7635977829, 2.6975179741; H, 2.0896722223, -0.5333190738, 2.2478452905; H, 5.6388370626, -0.4625604882, 1.1891825998; H, 5.2319669506, 0.2581559458, -0.3865286601; H, 5.1494514301, 1.2378109647, 1.0820473961; H, 1.9536262645, -3.0725093647, -0.3807091334; H, 2.5769469836, -3.4788180647, -2.7493506763; H, 2.1860712865, -1.7916151984, -2.3329985511; H, 3.8731724807, -2.3011665889, -2.46461071; H, 3.4909476, -4.9578353078, -0.9077882955; H, 4.7941695991, -

3.7976030114, -0.5861968528; H, 3.6778552466, -4.2404776771, 0.7099936634.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8634384 (hartree), -2668498.51833402 (kJ mol^{-1}).

TS15b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.3860796 (hartree), -3189470.51309027 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 4.634780364, -3.2114559626, 0.0898306749; C, 3.827558815, -4.308647078, -0.2056697707; C, 2.4649554482, -4.1350675058, -0.4412835447; C, 1.9305918759, -2.8608598603, -0.3769642407; C, 2.6959479675, -1.7202820095, -0.0819654324; C, 4.0614664713, -1.9541313423, 0.1457689558; N, 2.208289976, -0.4315628907, 0.0039910447; C, 1.0826415015, 0.0508980886, -0.1752769853; C, 0.0046052475, 0.682314378, -0.3303093778; C, -0.9582054489, 1.5686073876, -0.3821705511; O, -2.074585291, 1.9020868766, -0.5933401877; N, -0.0289381607, 3.3254228837, 0.2581159758; C, -0.3710104301, 4.3913680413, -0.6821503308; C, -0.5013466113, 3.5786044661, 1.6208246203; N, 3.0424984405, 2.8004295552, 0.2635259013; C, 3.6402126732, 3.2137348015, -1.0082331085; C, 3.7407896437, 3.3650327279, 1.4201862145; N, -4.6050741404, -0.1158307451, -1.291905794; C, -5.7626541046, 0.6415036906, -1.7584559584; C, -4.1438146896, -1.1051063643, -2.2632351709; N, -5.2017400073, -1.9567009814, 1.2974574162; C, -4.0694522124, -1.9189968715, 2.2095984988; C, -6.4653318761, -1.6469246699, 1.9461918744; F, 4.8440998705, -0.8909406152, 0.4323223921; H, 5.6956911191, -3.315816358, 0.2771375269; H, 4.2604883092, -5.2999318211, -0.2524449799; H, 1.8126813226, -4.9675311172, -0.6724509089; F, 0.6112616805, -2.6892024488, -0.6035719163; H, 0.9857219809, 3.1386617036, 0.2542010759; H, -0.0360753322, 5.3749696432, -0.3277010527; H, -1.4552857748, 4.4181739329, -0.8161124617; H, 0.092433141, 4.1882515756, -1.6489276635; H, -1.5933452211,

3.6197482848, 1.6244245869; H, -0.1157545535, 4.5261734854, 2.0191362279; H, -0.180908484, 2.7655599505, 2.274223633; H, 3.0740306518, 1.7846809451, 0.3207763381; H, 4.7155799999, 2.9870409375, -1.0754192214; H, 3.5171024407, 4.2931366212, -1.1404556071; H, 3.132176284, 2.7103987624, -1.8336226948; H, 3.6171211269, 4.4523627383, 1.4313754601; H, 4.8206129599, 3.1493189791, 1.4225912848; H, 3.3102374923, 2.9665727557, 2.3414773087; H, -5.039831498, -1.3207123485, 0.5158184185; H, -3.9787412847, -0.9692110084, 2.7703849947; H, -4.1526143221, -2.7264520447, 2.9459021464; H, -3.1419911678, -2.0715706159, 1.652329667; H, -6.4702642736, -0.6773039002, 2.4798386361; H, -7.2677160977, -1.6292972347, 1.2041613941; H, -6.7105379357, -2.4234454011, 2.6795676068; H, -3.8469636807, 0.5251415168, -1.0773231395; H, -3.931764222, -0.6772277834, -3.2579648074; H, -3.2357138971, -1.5864079015, -1.8946262037; H, -4.9053456167, -1.8810163621, -2.3863935017; H, -5.6019242643, 1.137770476, -2.7310061562; H, -6.6213727115, -0.0286166416, -1.8666212904; H, -6.0249586874, 1.4053145379, -1.0227194113.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.394232 (hartree), -3189491.906983 (kJ mol^{-1}).

TS15c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9024959 (hartree), -2710588.93043652 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.1006770631, 5.0629452762, -0.3349644524; C, 1.2907410014, 5.0907983033, -0.3392558267; C, 1.967660388, 3.8779442076, -0.2076134289; C, 1.243008523, 2.7019521992, -0.0816607915; C, -0.1608956015, 2.789271963, -0.0946259959; N, -0.8214667293, 3.9453480075, -0.2149699561; N, -0.9717443018, 1.6553922521, 0.0273292689; C, -0.6738260557, 0.4602456124, 0.0629087675; C, -0.4777908779, -0.7870102689, 0.0995282188; C, -0.6295393084, -2.0879330798, 0.1218756132; O, -0.1932643113, -

3.1921012132, 0.0837917725; N, -2.6607704579, -2.3465135592, 0.3736063671; C, -3.1190470765, -3.3477597201, -0.5886298252; C, -2.8751045426, -2.7399676321, 1.7679660518; N, -4.0240340813, 0.4082438336, -0.1488628304; C, -4.5169339537, 0.5174285978, -1.5238714047; C, -5.0546702679, 0.7277377288, 0.8408962691; N, 3.0096258846, -2.7498176034, -0.7613820013; C, 3.9419213167, -3.8155164605, -0.4033260405; C, 2.9589815738, -2.4976330776, -2.1995382961; N, 3.545210993, 0.0956603804, 0.7247300928; C, 3.2093119242, -0.0559344417, 2.1349895937; C, 4.9322415052, 0.4897934794, 0.5161907329; H, -0.6699286122, 5.983585246, -0.4321353392; H, 1.8219071428, 6.0295392046, -0.4398862788; H, 3.051656104, 3.8447704345, -0.2016309011; H, 1.7520369298, 1.748191656, 0.0318785531; H, -3.0927741815, -1.4273311492, 0.1868855889; H, -4.1641861421, -3.6347035285, -0.4148074794; H, -2.4912170288, -4.2382485031, -0.5057657724; H, -3.0256974707, -2.950362256, -1.6005008477; H, -2.2897848302, -3.6367004432, 1.9856572256; H, -3.9316991359, -2.9540955276, 1.9741148491; H, -2.5431111744, -1.9362892586, 2.4269972532; H, -3.2439734165, 1.0531126243, -0.0338285457; H, -4.9628023306, 1.4991501096, -1.7467161182; H, -5.2799596346, -0.2460405688, -1.7056933927; H, -3.6945563097, 0.3502791025, -2.2227000815; H, -5.849559236, -0.0237821775, 0.803138076; H, -5.5171803511, 1.7143969136, 0.6819860081; H, -4.6209131095, 0.7119277273, 1.8432170508; H, 3.3646306067, -0.7852912836, 0.2394023004; H, 3.8763410207, -0.7497659226, 2.6780042552; H, 3.2645927918, 0.9148428306, 2.639952346; H, 2.1846583443, -0.4229494622, 2.2298815526; H, 5.6644815937, -0.1901204243, 0.988551941; H, 5.1484886703, 0.5307426344, -0.5544211097; H, 5.103836641, 1.4899929826, 0.9295794197; H, 2.0790208629, -2.9915419777, -0.4328095057; H, 2.7223663058, -3.3953228455, -2.7954503758; H, 2.2073643124, -1.7342868587, -2.4113092013; H, 3.9276507613, -2.118702271, -2.5404454561; H, 3.7516817172, -4.7639298034, -0.933870243; H, 4.9648163486, -3.503759495, -0.636757643; H, 3.887889239, -4.0068673039, 0.6707759943.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9094977 (hartree), -

2710607.30487326 (kJ mol^{-1}).

TS15d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8985152 (hartree), -2710578.48410553 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, 0.3832630168, 5.1759297624, -0.4844491137; C, 1.7053875332, 4.9853508877, -0.4108092367; C, 2.2842263609, 3.7294454063, -0.2332336997; C, 1.4679106354, 2.6092433188, -0.1275716064; C, 0.0820312892, 2.7991578697, -0.2084640349; C, -0.4004309346, 4.104162434, -0.3838138499; N, -0.8563499339, 1.7627730704, -0.1190091207; C, -0.6731781009, 0.5441015716, -0.0517462867; C, -0.5979196613, -0.7141941663, 0.0146960715; C, -0.7709777802, -2.0083685051, 0.0781158718; O, -0.3690708434, -3.1252400306, 0.102901485; N, -2.8378379828, -2.2233290344, 0.1987372443; C, -3.2613738146, -3.0324380807, -0.9441424223; C, -3.1357728157, -2.8437764098, 1.490130014; N, -4.069433402, 0.6406931235, 0.0511529291; C, -4.8222575305, 0.8750432508, -1.1830153373; C, -4.8370695975, 0.9842302627, 1.2500341547; N, 2.8575156596, -2.9414022545, -0.6788832978; C, 3.7243273582, -4.0592637912, -0.3150196417; C, 2.8383074742, -2.6800635022, -2.1162651708; N, 3.5037879782, -0.1321313677, 0.8124001107; C, 3.1157337004, -0.2560168762, 2.2120971898; C, 4.9138011341, 0.1968613629, 0.6472750513; H, -1.4731200516, 4.2662784488, -0.4450072117; H, 2.3242778312, 5.8737540324, -0.4961513316; H, 3.3620778196, 3.6281059865, -0.1770280215; H, 1.9020611694, 1.6225396232, 0.0224657576; H, -3.2365882496, -1.2735259398, 0.1461109064; H, -4.3271606309, -3.2906799187, -0.8921454116; H, -2.6789623264, -3.9568125119, -0.9656529679; H, -3.0764530191, -2.4826456524, -1.8684236389; H, -2.5534856418, -3.7629999253, 1.5905496603; H, -4.2006469284, -3.091051537, 1.590964948; H, -2.8541794619, -2.1629476977, 2.2950769175; H, -3.2217165973, 1.2033705723, 0.0293307487; H, -5.2144867254, 1.9009645074, -1.2638044936; H, -5.6727558071, 0.188219689, -1.2331248893; H, -4.1815355136, 0.6848889085, -2.046685914; H, -5.6911449796, 0.3071143632, 1.3476157125; H, -5.225774832, 2.0145834155, 1.2365619538; H, -4.2091986385,

0.8671138161, 2.135960713; H, 3.2987839551, -1.0080834342, 0.3274010748; H, 3.7313729717, -0.9756562433, 2.7812877835; H, 3.2003318796, 0.7152742797, 2.7119066982; H, 2.072379251, -0.5737204462, 2.2765852433; H, 5.5979325311, -0.5138068529, 1.145390256; H, 5.1658507467, 0.2226594694, -0.4159220606; H, 5.1175590507, 1.1900067576, 1.0626958819; H, 1.9108586822, -3.1309888848, -0.36225306; H, 2.5587846055, -3.5601321112, -2.7197222007; H, 2.1334240701, -1.8745642806, -2.3326556798; H, 3.8306288885, -2.3544935643, -2.4438238731; H, 3.4866203318, -4.9936612038, -0.8511571813; H, 4.765595119, -3.805106815, -0.5365338773; H, 3.6481483937, -4.2506599007, 0.7577320145.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9059525 (hartree), -2710598.00140085 (kJ mol^{-1}).

TS15e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8996722 (hartree), -2710581.52035668 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -5.1933499595, -0.1192092085, -0.2631301249; N, -5.2150796721, -0.1414183783, 1.0738306876; C, -4.0272784508, -0.1549697324, 1.692521518; C, -2.7972813335, -0.1452256298, 1.0426226927; C, -2.7947708955, -0.1184690859, -0.3591675258; C, -4.0274551884, -0.1086877138, -1.0205150004; N, -1.6259015409, -0.1073211685, -1.129068664; C, -0.4500450349, -0.0214297207, -0.75931455; C, 0.7801511091, 0.0674025093, -0.4977154697; C, 2.0840422991, 0.1542276528, -0.4687965328; O, 3.1228622614, 0.2762348908, 0.0888386255; N, 2.6289154637, -0.0082337368, -2.4864307962; C, 3.3514431075, 1.2125671374, -2.8431698169; C, 3.4371351833, -1.220465663, -2.620923312; N, -0.0155482886, -0.2556490691, -4.1309137869; C, -0.2745452117, 0.9178565337, -4.9677706039; C, -0.0992292304, -1.5099555444, -4.8819507451; N, 2.4112566905, 1.0975898102, 3.2449540939; C, 3.4239572944,

0.8783505055, 4.2743319131; C, 1.9937264681, 2.4941051156, 3.144607198; N, -0.290091645, -0.6945661989, 3.5135401663; C, 0.041937457, -2.0857740169, 3.2338016732; C, -0.8768756346, -0.5107250261, 4.8346946216; H, -4.0636870383, -0.0904574341, -2.1029889835; H, -6.1608530699, -0.1094972672, -0.7578743744; H, -4.0563776404, -0.1749063187, 2.7783913039; H, -1.8772829684, -0.1681251895, 1.6222794438; H, 1.7524497141, -0.0884401187, -3.0233287874; H, 3.7765108499, 1.1585302676, -3.8540824864; H, 4.1654815897, 1.370214606, -2.1312718; H, 2.6735261899, 2.0661385099, -2.7913434837; H, 4.2602676861, -1.1861646978, -1.9029055521; H, 3.8576251673, -1.3245872969, -3.629810228; H, 2.8217326729, -2.0951151025, -2.4038409356; H, -0.6973451441, -0.2762321542, -3.3756308387; H, -1.2324147995, 0.8624051943, -5.5086427039; H, 0.521597881, 1.0248444295, -5.7108808506; H, -0.2831078574, 1.8171740786, -4.3482827983; H, 0.7047113076, -1.5503123839, -5.6231893834; H, -1.0543078945, -1.6336222587, -5.4163975155; H, 0.0244076225, -2.3557722008, -4.2021817185; H, 0.5523652575, -0.1225657616, 3.4308108187; H, 0.6985887667, -2.5474501463, 3.9933442403; H, -0.8730586064, -2.6860820263, 3.1828039942; H, 0.5402209193, -2.1562888234, 2.263889463; H, -0.2506546951, -0.8999059725, 5.6579443757; H, -1.0546970614, 0.5523011707, 5.0158249567; H, -1.8431309831, -1.024005295, 4.889830343; H, 2.7710900394, 0.7915299144, 2.3456314502; H, 2.8305503762, 3.1926550003, 2.9753177896; H, 1.2794215767, 2.6050964785, 2.3260724354; H, 1.4922602893, 2.7947230183, 4.0697950573; H, 4.3164832125, 1.5162158727, 4.1574491303; H, 2.9962436417, 1.0833043688, 5.2606491543; H, 3.744255979, -0.1658790746, 4.2597719649.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9076884 (hartree), -2710602.55682727 (kJ mol^{-1}).

Int5a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated

Energy E(HF) = -1016.8600181 (hartree), -2668489.54262977 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.1435182468, 2.9711181376, -0.0854115943; C, 1.9905344212, 2.1934335456, -0.046581782; C, 0.7303758584, 2.8128838674, -0.0895667369; C, 0.6558198484, 4.2106699357, -0.1667693392; C, 1.8158939002, 4.9779927848, -0.2041585179; C, 3.0671611374, 4.3628595672, -0.1646932085; N, -0.4810581175, 2.1000009909, -0.0559271256; C, -0.604092799, 0.8588961713, -0.0158707789; N, 3.473826502, -1.122113335, 0.7602314998; C, 3.1359478331, -1.0653290553, 2.1752034802; C, -0.8629010936, -0.3695798706, 0.0177950364; C, -1.4635524615, -1.5748221461, 0.0218758358; O, -1.1288135718, -2.7505692702, 0.0242810978; N, -3.0912352827, -1.4023958191, 0.0251356796; C, -3.6541308365, -2.029044533, -1.1965295512; C, -3.6467007491, -2.0002631256, 1.2647601791; C, 4.9011232975, -1.2832501068, 0.5262267705; N, 1.8588213977, -3.5354965031, -0.6405962042; C, 2.1082761261, -4.8816741698, -0.1372662731; C, 2.0387665201, -3.4281275555, -2.0845565121; N, -3.7820413513, 1.4696101468, -0.0691908079; C, -4.5999231164, 1.8611333166, -1.2227939597; C, -4.3259765094, 1.9757548582, 1.19686068; H, -0.3221432615, 4.677428273, -0.197039194; H, 1.7422501002, 6.0585501435, -0.2642891743; H, 3.9716688254, 4.9599253425, -0.1938679989; H, 4.1097958552, 2.4797224455, -0.0516014126; H, 2.0770697188, 1.1130860636, 0.0234794089; H, -3.3125821543, -0.3739120504, 0.0113081359; H, -4.7421744467, -1.9418495783, -1.1883607453; H, -3.3583188553, -3.0768188641, -1.218372185; H, -3.249852245, -1.5185907905, -2.070174203; H, -3.3499617127, -3.047094042, 1.310217466; H, -4.7349767484, -1.9147578654, 1.2605663905; H, -3.2380666196, -1.4686181855, 2.1235785605; H, -2.845568198, 1.8559172899, -0.1872086649; H, -4.7565466395, 2.9479212761, -1.2862839605; H, -5.582766056, 1.3844720602, -1.1595493526; H, -4.117903011, 1.5313681458, -2.1455204436; H, -5.2876491194, 1.4971900958, 1.4055494767; H, -4.4850414024, 3.0637912169, 1.1875361763; H, -3.6383716501, 1.7389364336, 2.011034019; H, 2.963798315, -1.8888896671, 0.3173806347; H, 3.5058568228, -1.9303440452, 2.7568829061; H, 3.5600608464, -0.1613529712, 2.6262789291; H, 2.0505817417, -1.0163974968, 2.2908863249; H, 5.3411134548, -2.1624694187, 1.0331567958; H, 5.0913391615, -1.3798091988, -0.5457833641; H, 5.4424861634, -

0.398903376, 0.8811337808; H, 0.9108025412, -3.2549879496, -0.3984305847; H, 1.4235476068, -4.1427344484, -2.6592541933; H, 1.7865795725, -2.4167985726, -2.4111813478; H, 3.0867124389, -3.6126128429, -2.3433650112; H, 1.5047138665, -5.6585613374, -0.6386657911; H, 3.1630760584, -5.1411258033, -0.2758453076; H, 1.8919478266, -4.9202742134, 0.9328414856.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8695215 (hartree), -2668514.48187713 (kJ mol^{-1}).

Int5b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.3901128 (hartree), -3189481.09719412 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 3.3579825537, -3.5745551562, -1.1373630056; C, 2.5487656315, -2.4602498976, -1.0039653179; C, 2.9897665909, -1.2429374352, -0.4548449025; C, 4.3329194704, -1.2358178937, -0.0387492234; C, 5.1756746862, -2.326019165, -0.1546786692; C, 4.6823895756, -3.505799702, -0.7096909486; N, 2.2343335359, -0.099082891, -0.2886298566; C, 1.0508103392, 0.1337676331, -0.6341726054; N, -4.3684725357, -1.3491629518, 2.3344893049; C, -3.1267097715, -0.9831407932, 2.9905020585; C, -0.101140238, 0.5368194938, -0.903902499; C, -1.2058181215, 1.3079557023, -1.0196112231; O, -2.3262617014, 1.2006770851, -1.4842932967; N, -0.9444557318, 2.7697934995, -0.3509734613; C, -1.0177899354, 3.8121280327, -1.4057209962; C, -1.9313295491, 3.0014720319, 0.7343713943; C, -5.4899596845, -0.514317446, 2.7282316104; N, -4.0518288522, -1.3864703844, -0.8538141543; C, -5.3840064091, -1.3594964294, -1.4495906427; C, -3.3083631054, -2.5996224876, -1.1872109681; N, 1.747747458, 2.9165853079, 0.8507586567; C, 2.5859745309, 3.9785984435, 0.2810402115; C, 1.7029157071, 2.9716265573, 2.317496741; F, 4.8199625895, -0.0948923916, 0.5017056689; H, 6.1988951818, -2.2392283034, 0.187840052; H, 5.3281251529, -4.3693289085, -0.8079717038; H, 2.9424349597, -

4.4752646994, -1.571268297; F, 1.2646661203, -2.5364145798, -1.4185801015; H, 0.0259169237, 2.7738669331, 0.0632378177; H, -0.8658134018, 4.7965122612, -0.9598289083; H, -1.9958414484, 3.7602147439, -1.882068636; H, -0.2409816767, 3.6180356761, -2.1446657319; H, -2.9342106122, 2.9299158578, 0.3165945341; H, -1.7708018092, 3.9891438665, 1.1699642835; H, -1.8017413769, 2.2349009341, 1.4976450749; H, 2.1437588105, 2.0157697348, 0.5790004597; H, 3.6031238996, 3.9876958598, 0.6982020308; H, 2.13348262, 4.9554855095, 0.4772626731; H, 2.6624347556, 3.8465010465, -0.8002422565; H, 1.1999819663, 3.8883860205, 2.6399906023; H, 2.7028786874, 2.9561507148, 2.7740395151; H, 1.1398499502, 2.1178909351, 2.69978953; H, -4.2514613293, -1.3314240491, 1.3189901656; H, -2.8496050635, 0.0831355955, 2.8626129608; H, -3.1991232655, -1.1695597761, 4.0681081656; H, -2.3076486978, -1.5925343662, 2.6014852917; H, -5.3178247417, 0.5697190249, 2.5780561201; H, -6.3789468804, -0.7962070806, 2.1586988667; H, -5.7157882809, -0.6630623901, 3.7903141972; H, -3.5248132044, -0.5733242156, -1.1629513611; H, -3.2529841338, -2.7933644662, -2.27175977; H, -2.2887279111, -2.5229938401, -0.8045177216; H, -3.7836500147, -3.4653270578, -0.7150760735; H, -5.3789872346, -1.4959244161, -2.5447572684; H, -5.9978336574, -2.1574640563, -1.0191800771; H, -5.8694236897, -0.4060780216, -1.2269877783.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.4020598 (hartree), -3189512.44904589 (kJ mol^{-1}).

Int5c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9057276 (hartree), -2710597.41120821 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 2.4269286053, 3.5515284762, -0.2400388297; C, 1.5215360345, 2.5087154428, -0.1191971074; C, 0.1469896749, 2.8116905633, -0.1652666935; N, -0.3157310414, 4.0603558311, -0.3110549776; C, 0.5767195374,

5.0467910621, -0.4256163856; C, 1.9548570718, 4.8552715437, -0.3996078941; N, -0.8407019843, 1.8284323305, -0.0526343546; C, -0.6715775008, 0.5930102772, -0.004581285; N, 3.5551626932, -0.3450731951, 0.7922905507; C, 3.1468692024, -0.4624684207, 2.1855113799; C, -0.6377494504, -0.6606740283, 0.0440200905; C, -1.067754971, -1.9383579693, 0.1170064914; O, -0.5701784166, -3.0523647137, 0.1037591445; N, -2.6922356588, -1.9830539344, 0.2730606052; C, -3.2772426208, -2.8046283529, -0.8151612911; C, -3.0378386932, -2.5088088201, 1.6178022082; C, 4.9938621656, -0.1842975978, 0.6377914685; N, 2.5092113055, -2.9630160458, -0.7824808699; C, 3.2101192414, -4.2196687578, -0.5406365281; C, 2.447485071, -2.6106423833, -2.1977157529; N, -3.8592187621, 0.7186838539, 0.0435939008; C, -4.5506051418, 0.9188205722, -1.2362122498; C, -4.6945479092, 1.096849583, 1.1897105699; H, 0.163389577, 6.0453559111, -0.5439158255; H, 2.6301020531, 5.6968145101, -0.4974116631; H, 3.491276049, 3.3453229612, -0.2074792431; H, 1.8729411696, 1.4899904723, 0.0161412164; H, -3.059071244, -0.9964146249, 0.1897951352; H, -4.3597528954, -2.8635262481, -0.6891724627; H, -2.8356868192, -3.799249001, -0.7783085488; H, -3.0429853096, -2.3380562337, -1.7715144949; H, -2.6066304625, -3.5031006409, 1.7273514371; H, -4.1227804079, -2.5535025499, 1.7280592869; H, -2.6182846814, -1.8434961757, 2.3716869479; H, -3.0248230462, 1.3084062669, 0.0459339341; H, -4.9313076928, 1.942956725, -1.357261096; H, -5.3997308175, 0.2324758342, -1.3129845094; H, -3.8639612059, 0.7123041856, -2.0596282592; H, -5.5539757538, 0.4231212472, 1.2631976998; H, -5.0770659606, 2.124983534, 1.1162639289; H, -4.1138644395, 1.0150938067, 2.1109360057; H, 3.2431683014, -1.1720282564, 0.2784271984; H, 3.6697391312, -1.266466401, 2.7356491119; H, 3.3411389544, 0.4772016496, 2.7147574797; H, 2.073124389, -0.6575272015, 2.2359175883; H, 5.5869690904, -0.9857638665, 1.1159760808; H, 5.2514714916, -0.1598900322, -0.4242492893; H, 5.3148162478, 0.7654866292, 1.0803524989; H, 1.5620647446, -3.0271177731, -0.4154676664; H, 2.0016023198, -3.3997769421, -2.8279519495; H, 1.8606001409, -1.6979635484, -2.3206016882; H, 3.4563989359, -2.4157462514, -2.5760907838; H, 2.7959981192, -5.0715841675, -1.1076564034; H, 4.2637959784, -4.1169630251, -0.8201758453; H, 3.1690436099, -4.4655121091, 0.5230778931.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9171144 (hartree), -2710627.29295809 (kJ mol^{-1}).

Int5d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9019976 (hartree), -2710587.62277537 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.6837841219, -0.0406699325, -4.2747216701; C, 0.624135235, -0.0430197639, -2.8858510618; C, 1.83050026, 0.0054877039, -2.1730329872; C, 3.0257088075, 0.0468110793, -2.9088163149; N, 3.0829003339, 0.0486871353, -4.239136024; C, 1.9246879375, 0.0067410901, -4.9083006579; N, 1.9302763467, 0.0085752222, -0.7755312018; C, 0.9773842314, 0.0366855309, 0.0324257592; N, -2.8098038457, -0.76601868, -2.1965350958; C, -2.6784567415, -2.1777761308, -1.8627489436; C, 0.1136785605, 0.0662583976, 0.941222982; C, -0.5057671538, 0.1118781123, 2.1381332613; O, -1.6525825825, 0.1763915314, 2.553330176; N, 0.589546937, 0.0676417132, 3.3450963089; C, 0.4952177347, 1.3163400708, 4.1424470871; C, 0.3624749809, -1.1428003923, 4.1738686732; C, -3.7030660794, -0.5338589496, -3.322990599; N, -3.8928983844, 0.8192212571, 0.390680153; C, -5.2091701717, 0.4239555109, 0.8810142814; C, -3.7943455231, 2.2507764239, 0.1234422454; N, 3.3244255384, -0.1059119682, 2.2384789257; C, 4.2244248541, 0.968035339, 2.6756323945; C, 3.9144209868, -1.4375332106, 2.4249937095; H, 3.9702543042, 0.0805764618, -2.3721928866; H, 1.9947803443, 0.0090916586, -5.9922340615; H, -0.2278600509, -0.077946288, -4.8603060538; H, -0.3378595329, -0.0916422723, -2.3812242376; H, 1.5491464384, 0.0107739298, 2.9129559289; H, 1.2074879681, 1.2801094452, 4.9685848083; H, -0.520827906, 1.4118050026, 4.5224910646; H, 0.72344332, 2.1630213475, 3.4957097886; H, -0.6564397371, -1.1173326406, 4.5573052048; H, 1.077533641, -1.1638205642, 4.9981236314; H, 0.4942119543, -2.0251323364, 3.5484587027; H, 3.1314555501,

0.016902017, 1.2440562473; H, 5.2114471363, 0.9207780824, 2.1932456737; H, 4.3773285598, 0.9068567228, 3.7573322372; H, 3.7788026374, 1.938378422, 2.4467524531; H, 4.0402698117, -1.6419058523, 3.4925935593; H, 4.8977947698, -1.5387897565, 1.9438538122; H, 3.2497300837, -2.194568951, 2.0043168626; H, -3.1495891406, -0.2544182261, -1.3789714928; H, -3.6442127834, -2.6820198359, -1.6747163281; H, -2.1832968161, -2.7125097277, -2.6809342249; H, -2.0582063075, -2.2867333605, -0.9697987421; H, -4.711860493, -0.9660124158, -3.1888060903; H, -3.8140206842, 0.5403902637, -3.4912783108; H, -3.2805687459, -0.9714417227, -4.2345480288; H, -3.1854982817, 0.5582108678, 1.0744881371; H, -4.0566844569, 2.8793815511, 0.9922242051; H, -2.7754138557, 2.4964495461, -0.1838133248; H, -4.4672535271, 2.5230068778, -0.6963814652; H, -5.5331704806, 0.985428725, 1.7745666342; H, -5.9599349362, 0.5825329156, 0.0999271852; H, -5.2051288502, -0.6397801684, 1.1298972855.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.913739 (hartree), -2710618.43508243 (kJ mol^{-1}).

Int5e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9034501 (hartree), -2710591.43449084 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.7040668663, -0.04174376, -4.2630057982; C, 0.6518274597, -0.0405836465, -2.8732631719; C, 1.861292322, 0.0113253416, -2.1631271864; C, 3.0487486148, 0.0528393886, -2.9053976553; C, 2.9778317213, 0.0470148536, -4.2932401701; N, 1.8327535807, 0.001803011, -4.9838463828; N, 1.9541789511, 0.0162599667, -0.7670325099; C, 0.9911136326, 0.0534183749, 0.0320510835; N, -2.8072893599, -0.7761253647, -2.1818343754; C, -2.67635879, -2.1899323817, -1.8585214263; C, 0.1245531849, 0.0937556247, 0.9353288574; C, -0.501012314, 0.1265207189, 2.1312734362; O, -1.648462652,

0.19374319, 2.5394158119; N, 0.5871040871, 0.0607413628, 3.3415527937; C, 0.5042414776, 1.3056806655, 4.1466163997; C, 0.3412914876, -1.1523567846, 4.1615756758; C, -3.6681998698, -0.5371605683, -3.3316767645; N, -3.9262682192, 0.8175662896, 0.3931056934; C, -5.2493022826, 0.4489839608, 0.885435545; C, -3.8058314215, 2.2424132442, 0.1005011322; N, 3.3240203391, -0.1266003962, 2.2530894457; C, 4.210458294, 0.9645185397, 2.6754656509; C, 3.9260542014, -1.4484505428, 2.468566609; H, 4.0039305197, 0.0905014126, -2.3951922332; H, 3.8907825908, 0.0803628063, -4.8823342014; H, -0.2218233202, -0.0815974453, -4.8301592386; H, -0.3113012694, -0.0912343097, -2.3726575051; H, 1.5488817437, -0.0048000453, 2.9140405015; H, 1.2151409288, 1.2565595557, 4.9731811456; H, -0.5110886001, 1.4092666459, 4.5264253552; H, 0.7420671834, 2.1540071511, 3.5055500278; H, -0.6784652331, -1.1163768974, 4.5417421497; H, 1.053318598, -1.1874974631, 4.9878770252; H, 0.4640560272, -2.0322919059, 3.5309457691; H, 3.1359747329, -0.0234325098, 1.2553675356; H, 5.2011664211, 0.9175091569, 2.2006737439; H, 4.3566447226, 0.9258396979, 3.7591092205; H, 3.7570355572, 1.9256807363, 2.4244344563; H, 4.0480542211, -1.6310522664, 3.5405011471; H, 4.9131662468, -1.5491196732, 1.9949372698; H, 3.2714276381, -2.220410998, 2.059301405; H, -3.1699366254, -0.2728512218, -1.3695488045; H, -3.6435640873, -2.7026603337, -1.7025089244; H, -2.1547908452, -2.7130128056, -2.6676589953; H, -2.0802221849, -2.3042079169, -0.9498110146; H, -4.6781742031, -0.9760024069, -3.2316371697; H, -3.7797182648, 0.5381207757, -3.4925527823; H, -3.2162001429, -0.9626911021, -4.2345435115; H, -3.2233758325, 0.5573889499, 1.0813773688; H, -4.0613156592, 2.890612579, 0.9568968346; H, -2.7826947548, 2.467229109, -0.2085459524; H, -4.4723052973, 2.5091900527, -0.726232832; H, -5.5688818907, 1.0297132666, 1.7683228626; H, -5.9949960053, 0.6048787215, 0.0990519185; H, -5.2612348566, -0.6105390906, 1.1515849773.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.916156 (hartree), -2710624.77788194 (kJ mol^{-1}).

TS25a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8500721 (hartree), -2668463.4418917 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0, -3.069034017, -0.4673060307, 2.8515169872; C, 0, -3.0688277358, -0.4519736217, 4.2428207088; C, 0, -1.8644553524, -0.4394866955, 4.9465835456; C, 0, -0.6612306989, -0.4457591795, 4.2385747361; C, 0, -0.6484660156, -0.4604560878, 2.8471833193; C, 0, -1.8616256915, -0.4673306651, 2.13694147; N, 0, -1.9348035732, -0.4782422578, 0.733824017; C, 0, -0.9476982749, -0.4152351692, -0.0504186274; C, 0, -0.1050971653, -0.3070723551, -0.965999453; C, 0, 0.3529028586, 0.0552805878, -2.2092444676; N, 0, -0.7927732345, 0.0268355755, -3.2395232455; C, 0, -1.0371331005, -1.3668535141, -3.6835518168; O, 0, 1.4615325506, 0.3848855531, -2.6206468781; C, 0, -0.5022175448, 0.9040446686, -4.3921189796; N, 0, -2.9156791843, 0.8087828889, -1.8897787639; C, 0, -4.1824429146, 0.4629677674, -2.5670217531; C, 0, -2.7811105381, 2.2544730368, -1.5996697763; N, 0, 3.735269606, 0.9261311901, -0.512206729; C, 0, 3.56457654, 2.2963864332, -0.0426263229; C, 0, 5.0316630723, 0.7008777628, -1.1411626684; N, 0, 2.8948304853, -1.0406542873, 1.9177315077; C, 0, 3.9283191334, -1.0343844571, 2.9422444573; C, 0, 2.6311873432, -2.3716131336, 1.3890995321; H, 0, -4.000965959, -0.4844790733, 2.2970075605; H, 0, -4.0121045514, -0.452829146, 4.7788295297; H, 0, -1.8629526343, -0.4292925658, 6.0306780191; H, 0, 0.2833378136, -0.4409702076, 4.7719624244; H, 0, 0.3020916119, -0.4730759912, 2.3210787297; H, 0, -1.9126148484, 0.4359975042, -2.5582615539; H, 0, -1.3593629234, 0.8927286806, -5.0704461589; H, 0, 0.3911308723, 0.572514678, -4.9248094724; H, 0, -0.3286211304, 1.9215331395, -4.0420667021; H, 0, -0.1516656753, -1.7741639125, -4.1813818381; H, 0, -1.8761763049, -1.3861313823, -4.3842383306; H, 0, -1.273147438, -1.98401431, -2.81726722; H, 0, -2.8605350646, 0.3055268236, -0.9910375985; H, 0, -3.6096197937, 2.6067078412, -0.9803797753; H, 0, -2.7713832569, 2.8148263527, -2.536349775; H, 0, -1.8436735447,

2.4190960594, -1.0692207313; H, 0, -4.2196176267, 0.9463705856, -3.5452059647; H, 0, -5.0437496325, 0.7901740975, -1.9785696758; H, 0, -4.2362780198, -0.6177825853, -2.7006331276; H, 0, 3.1636339749, -0.4176812029, 1.153375614; H, 0, 3.5334886326, -2.8850517616, 1.0073554984; H, 0, 2.1984759325, -3.0065738124, 2.1704854971; H, 0, 1.9064092011, -2.3032381251, 0.5747093516; H, 0, 4.8828447916, -1.4887200923, 2.6163461331; H, 0, 4.1320021388, -0.0074003637, 3.2566036204; H, 0, 3.5874027417, -1.5904005852, 3.8229638018; H, 0, 2.9956418005, 0.7040153492, -1.176883571; H, 0, 3.7098647535, 3.0546454492, -0.832470487; H, 0, 2.5613805481, 2.4190806388, 0.371863172; H, 0, 4.2843131704, 2.5084798998, 0.7551540456; H, 0, 5.2472867386, 1.3994335812, -1.9687706981; H, 0, 5.8303146316, 0.8093779533, -0.3995392229; H, 0, 5.0768205611, -0.3171157908, -1.5349389227.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8621676 (hartree), -2668495.18344381 (kJ mol^{-1}).

TS25b

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.3810581 (hartree), -3189457.33544537 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.219116707, 0.6624913056, -0.0164118159; C, -0.2684256965, 0.2047622318, 1.3128161231; C, 0.9617959297, -0.2491830935, 1.8206489897; C, 2.1387547799, -0.2554028628, 1.0962210214; C, 2.125221151, 0.2107822457, -0.2180062631; C, 0.9358970902, 0.6729413208, -0.7783072669; N, -1.387429986, 0.1425261018, 2.1169370763; C, -2.5325015509, 0.6574675476, 1.9323001019; C, -3.692160876, 1.1010809943, 2.001116387; C, -4.8814133491, 1.4200158499, 2.6195531111; N, -5.0396610964, 0.6247589322, 3.9302268071; C, -5.581583267, -0.7231121575, 3.6228951491; F, 0.9848926535, -0.6995049813, 3.1020746355; F, -1.3693699838, 1.1050939436, -0.5733294188; O, -5.7854791456,

2.1889151961, 2.3250705038; C, -5.9111612572, 1.3380548731, 4.8878789942; N, -2.6119299327, 0.2640468276, 4.8840013193; C, -2.5517735324, -0.8274589744, 5.8783898977; C, -2.1016048804, 1.5528273307, 5.4030079936; N, -6.761732505, 2.7536683582, -0.6143352991; C, -5.6712913085, 3.0996408928, -1.5213099291; C, -7.8179476671, 3.7601640507, -0.5902666852; N, -8.1696782672, -0.0062705551, -1.4421763632; C, -8.7300150322, -0.6367007393, -0.2600825221; C, -7.2599807614, -0.8748883232, -2.1716477056; H, 3.0440411401, -0.6207478179, 1.5642406596; H, 3.0368010908, 0.2134474898, -0.802039875; H, 0.8878024681, 1.0397029193, -1.7959554871; H, -3.7955489365, 0.4384720012, 4.4374712835; H, -5.9666198122, 0.7598590504, 5.8135398428; H, -6.9140223579, 1.4747317576, 4.4798321154; H, -5.4918612411, 2.3219906465, 5.0985596054; H, -6.5681531493, -0.6450073061, 3.1569474725; H, -5.6695762281, -1.2996492627, 4.547197532; H, -4.9048475102, -1.2346935663, 2.9390390875; H, -2.0343783164, 0.0088549275, 4.0682274812; H, -1.0675359025, 1.4546249778, 5.7424792886; H, -2.7222411272, 1.8818353891, 6.2387265255; H, -2.1468580339, 2.2954215119, 4.6066486119; H, -3.1999691405, -0.5903434815, 6.7244323554; H, -1.5310314455, -0.9689625103, 6.2432607647; H, -2.8920890181, -1.7549053988, 5.4170392394; H, -7.6954783446, 0.8617431207, -1.1829122892; H, -6.4319797572, -1.2749399626, -1.556213085; H, -7.8066251721, -1.7317097763, -2.5821085732; H, -6.8223059105, -0.3290547254, -3.0110558087; H, -7.9683806855, -1.0323020327, 0.4407857179; H, -9.3486166123, 0.0816824165, 0.2839567784; H, -9.3722291215, -1.4767053041, -0.5491946153; H, -6.3923096646, 2.6274601694, 0.3255703601; H, -5.2372225453, 4.0952213364, -1.3246087222; H, -4.8736413488, 2.3587110107, -1.4369309696; H, -6.0328866537, 3.093826519, -2.5550351788; H, -7.4517546369, 4.7759584925, -0.3600476226; H, -8.3167021551, 3.7977164118, -1.5641427168; H, -8.5672563326, 3.4902228294, 0.1575946384.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.395176 (hartree), -3189494.38427003 (kJ mol^{-1}).

TS25c

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.897415 (hartree), -2710575.59691148 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.0490776458, 0.1481070268, -0.1116537631; N, -0.0276414422, 0.3304083015, 1.2152319927; C, 1.1118905674, 0.33676156, 1.9120157283; C, 2.3711568744, 0.1635171866, 1.346924845; C, 2.4410623473, -0.0265752319, -0.0348686747; C, 1.2749434429, -0.0369604152, -0.7833058199; N, -1.177585135, 0.145788922, -0.775980663; C, -1.3531338187, 0.1624464727, -2.0254564319; C, -1.7301677123, 0.2339653735, -3.2130040317; C, -2.6240986603, 0.5631418912, -4.2042057791; O, -2.479250642, 0.8504417239, -5.3866397926; N, -4.0696026694, 0.5494369386, -3.6603854431; C, -4.9487778405, 1.4357847953, -4.4518162924; C, -4.5853744179, -0.8418802458, -3.6552895695; N, -3.9289732154, 1.3210966699, -1.1443985405; C, -3.685950581, 2.7797853095, -1.097874589; C, -5.1108941925, 0.9066643077, -0.361206092; N, 0.5915871302, 1.355833766, -6.082805323; C, 0.8422083932, 1.3056405805, -7.5191352738; C, 0.8584035696, 2.670044824, -5.5076835903; N, 2.1570944547, -0.7763780248, -4.2131070123; C, 1.572168046, -2.0978156906, -4.3961161348; C, 3.5787622236, -0.7404265597, -4.524752811; H, 1.0080865292, 0.4881844395, 2.9837950924; H, 3.2601979047, 0.1760897538, 1.9658465657; H, 3.3970328944, -0.1669583065, -0.5280616694; H, 1.3126578204, -0.1868957347, -1.8590283099; H, -4.0107827214, 0.9468344892, -2.3789200338; H, -5.9479218337, 1.4299988129, -4.0089652043; H, -5.005041203, 1.1063542019, -5.4906787045; H, -4.5505394939, 2.4502578328, -4.4374084918; H, -4.6146751612, -1.2444362473, -4.6721041463; H, -5.5958972022, -0.8547657015, -3.2391585181; H, -3.932926405, -1.4637819472, -3.0432741633; H, -3.0911773841, 0.8567329535, -0.7572509458; H, -3.5549785425, 3.1216317944, -0.0680463014; H, -4.531321288, 3.3070497894, -1.5446801683; H, -2.7816564957, 3.0049064497, -1.6629801723; H, -6.0124485467, 1.3483183276, -0.7911603335; H, -5.0231023088, 1.2268678914, 0.6806022145; H, -5.1982771174, -0.1799401706, -0.3873817846; H, 1.6601528494, -0.1025149324, -4.7999441056; H, 1.7391551699, -

2.5212109179, -5.4037378626; H, 1.9974790297, -2.8004002199, -3.6705038746; H, 0.4951519583, -2.0462786059, -4.2209235375; H, 3.8231403309, -1.10307679, -5.540473168; H, 3.9519219256, 0.2829174852, -4.4324363579; H, 4.1347870767, -1.3630248308, -3.8145774097; H, -0.3786918456, 1.1054315993, -5.9000293164; H, 0.2972260108, 3.4860877315, -5.9959732381; H, 0.6020004582, 2.661950766, -4.4460843992; H, 1.9247422433, 2.9043457455, -5.5939929688; H, 0.2886588858, 2.0714698208, -8.0901612013; H, 1.9094536042, 1.4528484117, -7.7157722679; H, 0.5629378865, 0.3234486585, -7.9074944307.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.910378 (hartree), -2710609.6149959 (kJ mol^{-1}).

TS25d

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8924294 (hartree), -2710562.51347696 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.0419068903, -0.0003535478, -0.0590077073; C, 0.0775667323, 0.0340626078, 1.3450395871; N, 1.1972408259, 0.0407951817, 2.0655205946; C, 2.3601780691, 0.0069332456, 1.403598505; C, 2.4373676833, -0.0357586175, 0.0123179257; C, 1.2680944314, -0.0404800396, -0.7397837027; N, -1.2133287951, 0.0034800282, -0.6792996203; C, -1.4074673529, 0.0665648212, -1.9261317194; C, -1.7831505254, 0.1762332169, -3.1109547123; C, -2.6221599758, 0.5625754425, -4.129053662; O, -2.4124145991, 0.898204157, -5.2901218977; N, -4.0875277168, 0.5558918004, -3.6568243724; C, -4.9241580415, 1.4504379413, -4.4836150008; C, -4.6173585855, -0.8297680029, -3.6733137598; N, -3.9817399369, 1.3264095963, -1.1402502592; C, -3.6557660776, 2.7703663914, -1.10216483; C, -5.2052176074, 0.983407695, -0.385371777; N, 0.5841251321, 1.3788184714, -6.1559567669; C, 0.7214375892, 1.129181108, -7.5866966833; C, 0.9162071271, 2.7506768878, -5.7872670966; N, 2.1857327967, -

0.6138605657, -4.1762968126; C, 1.6188584003, -1.950018164, -4.301615346; C, 3.6102066721, -0.5751509822, -4.4756557094; H, -0.8618943539, 0.0552037733, 1.8922441575; H, 3.2607549518, 0.0120717183, 2.010758796; H, 3.4029474979, -0.0665322808, -0.4801552333; H, 1.3149623514, -0.0806906255, -1.8258399891; H, -4.0577982767, 0.9581097304, -2.3506974007; H, -5.9410143489, 1.4533927098, -4.0828807666; H, -4.9413510984, 1.1229206358, -5.5247253829; H, -4.5179820303, 2.4613276024, -4.453610505; H, -4.6103719343, -1.2328609527, -4.6906400809; H, -5.6444588284, -0.8327721196, -3.2991800858; H, -3.9969098643, -1.4596608577, -3.036763219; H, -3.1813934826, 0.8165412938, -0.7387016777; H, -3.533872427, 3.1160647126, -0.0727804759; H, -4.4585526688, 3.3374765232, -1.5768231453; H, -2.7260985897, 2.9347215592, -1.646331662; H, -6.0671911184, 1.4739877587, -0.8415826669; H, -5.1262984423, 1.3049663346, 0.6564609696; H, -5.3537832498, -0.0964018192, -0.4110838754; H, 1.6862698837, 0.0251331343, -4.7988794274; H, 1.8046269453, -2.419917954, -5.284987238; H, 2.0428678788, -2.6109657895, -3.5371712855; H, 0.5391403393, -1.9036292946, -4.1422441238; H, 3.8683164054, -0.9849332348, -5.4697516885; H, 3.9701635705, 0.4559995276, -4.4304843205; H, 4.1663726338, -1.1550835295, -3.7304774875; H, -0.3725860525, 1.1769119942, -5.8697415283; H, 0.3304577737, 3.5088687162, -6.3363365615; H, 0.7468995069, 2.8938489671, -4.7175847472; H, 1.9755785829, 2.9433109541, -5.9871471806; H, 0.1387031614, 1.8268346615, -8.2132961933; H, 1.7724386231, 1.2177489717, -7.8816053979; H, 0.3943148443, 0.1122466249, -7.8151575807.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9067641 (hartree), -2710600.13123787 (kJ mol^{-1}).

TS25e

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8942432 (hartree), -2710567.27333204 (kJ mol^{-1}). Structure definition (3D

Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 0.0037681885, -0.0203635603, -0.03203689; C, 0.0473740441, 0.0000643236, 1.3696208422; C, 1.2804798734, -0.0048669766, 2.0094418607; N, 2.4565364374, -0.0311172926, 1.3712986714; C, 2.4032649278, -0.0577453433, 0.0322308856; C, 1.2308767343, -0.0549984215, -0.7152113948; N, -1.2447352509, -0.0093364759, -0.6584632505; C, -1.4260873687, 0.0578529987, -1.9096769149; C, -1.7951074936, 0.1726128091, -3.0942832489; C, -2.6291785319, 0.5595944865, -4.1183102274; O, -2.4116197854, 0.8989406367, -5.275176715; N, -4.0962676148, 0.5521259063, -3.654562097; C, -4.9321038105, 1.4371220965, -4.4927614398; C, -4.6218613358, -0.835737244, -3.6600100397; N, -4.0020584738, 1.339410536, -1.1439385728; C, -3.6574318256, 2.7792682704, -1.1120996067; C, -5.2357361671, 1.0175624857, -0.3965667451; N, 0.5871108474, 1.3801169203, -6.1711052005; C, 0.7176925702, 1.1307164532, -7.6023786701; C, 0.9237139475, 2.7508196454, -5.8023627239; N, 2.1791003698, -0.6064137823, -4.1697606258; C, 1.6361150904, -1.9498905123, -4.315596192; C, 3.6122149358, -0.5459214916, -4.419023059; H, -0.8750246414, 0.015655605, 1.9388622493; H, 1.3264545742, 0.0120499644, 3.0956125643; H, 3.3607374161, -0.0829081975, -0.481159893; H, 1.2845054408, -0.0858388513, -1.8005330609; H, -4.0735008911, 0.9630379432, -2.3565690634; H, -5.9503239076, 1.4406068975, -4.09581415; H, -4.9444702764, 1.099917513, -5.5307704388; H, -4.5286916273, 2.4492208264, -4.4703673998; H, -4.6098455493, -1.2478465331, -4.6735307038; H, -5.6502293795, -0.8378043017, -3.2897710839; H, -4.002039211, -1.4577964699, -3.015291647; H, -3.2116422334, 0.8216056025, -0.7333313566; H, -3.5410467283, 3.130430362, -0.0838836821; H, -4.4481207386, 3.3537530428, -1.598088229; H, -2.7204189007, 2.9281470791, -1.6480354663; H, -6.0875900861, 1.516452512, -0.8626905799; H, -5.1612408274, 1.3451330019, 0.643785123; H, -5.398691749, -0.0603274603, -0.4162507048; H, 1.6906204585, 0.0277681897, -4.8051632593; H, 1.8591547197, -2.4152175481, -5.2936061103; H, 2.0453033516, -2.6061507294, -3.5392627356; H, 0.5513147375, -1.9199389066, -4.1896083151; H, 3.9114527699, -0.9476766308, -5.4049962609; H, 3.9552313087, 0.4900822585, -4.3570480249; H, 4.1500462293, -1.1203265223, -3.6565192079; H, -0.3675863706, 1.1786173255, -5.8792919447; H, 0.3371301542, 3.5110378566, -6.3478349275; H, 0.7601743725,

2.8929570137, -4.7316609083; H, 1.9825254045, 2.9411727908, -6.0069106528; H, 0.1330673601, 1.8290889893, -8.2265274461; H, 1.767501137, 1.2183949707, -7.9015128782; H, 0.3890308022, 0.1140044843, -7.829670338.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9096251 (hartree), -2710607.63920204 (kJ mol^{-1}).

TS16a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8454013 (hartree), -2668451.18456942 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.632746626, -0.6000320086, 0.6878670003; C, -2.650981691, 0.2671913847, 0.1773616879; C, -2.9960184866, 1.1277687552, -0.8773707937; C, -4.2684278731, 1.0824578783, -1.4368572543; C, -5.2308560713, 0.1993333143, -0.9447982725; C, -4.9063001679, -0.6328931205, 0.1257869729; N, -1.3940034097, 0.3624391591, 0.7619090156; C, -0.5029579478, -0.4771313565, 1.034989899; C, 0.5534246985, -0.569441965, 1.8566563763; C, 1.6306736286, -1.0817606445, 2.2666011104; N, 2.6383445021, 1.8140596523, -1.2891727698; C, 2.4505558506, 2.4823294994, -2.5699564411; O, 2.6516841995, -1.5120995423, 2.6932001545; C, 3.9936366362, 1.9628887905, -0.7729725329; N, 0.6032812369, 3.0800179981, 0.8875718374; C, -0.0895637214, 4.2917299677, 0.4604784451; C, 1.3078273959, 3.2515032875, 2.1569943736; H, -2.2507164447, 1.8191039206, -1.2527242701; H, -4.5124273757, 1.7461761241, -2.2591541745; H, -6.2233091933, 0.1723006317, -1.3789715061; H, -5.6522461017, -1.3054041929, 0.5356975449; H, -3.3952480002, -1.2209697056, 1.5438213539; H, 1.974508645, 2.1897255945, -0.6077746726; H, 4.3254543058, 3.0137450457, -0.6942210799; H, 4.703942814, 1.4446120941, -1.4271110625; H, 4.0624577878, 1.5106122418, 0.2191278334; H, 3.0617571235, 1.9979771968, -3.3399025755; H, 2.7237971378, 3.5530205772, -2.5583319901; H, 1.404770299,

2.4041567639, -2.8785367659; H, -0.0649013604, 2.3176776589, 0.9760189523; H, 0.6614826945, 3.6300406863, 2.9666346983; H, 2.1312527704, 3.9617176559, 2.0289140428; H, 1.7250670982, 2.294258586, 2.4733746383; H, 0.6411472503, 5.0774720276, 0.2431100449; H, -0.7910708324, 4.6876491463, 1.2144293063; H, -0.6500563558, 4.0962583891, -0.4571152791; N, -0.5012798243, -2.0240073915, -0.0080504869; H, 0.5287433344, -2.1492427684, -0.108342539; C, -1.0185956426, -3.1897935623, 0.733478066; C, -1.0481282835, -1.9158990133, -1.3757697769; H, -0.7172012185, -2.7728024864, -1.9729932404; H, -2.1353685283, -1.8927373203, -1.3520067028; H, -0.679346263, -1.000300602, -1.8365710023; H, -0.7306567779, -4.1201761722, 0.2328857984; H, -0.5991720961, -3.1832014038, 1.7395524111; H, -2.1056616804, -3.1388642525, 0.7907989165; N, 2.4012258108, -2.5735727374, -0.5484380135; H, 2.8573037958, -2.204070434, 0.281831241; C, 2.734537497, -3.9967024489, -0.6634520941; C, 2.8390587257, -1.7921005904, -1.7140143077; H, 3.8031312298, -4.1733673524, -0.859047871; H, 2.4644623031, -4.5165298417, 0.2584351006; H, 2.1682909072, -4.4420662957, -1.4871202219; H, 3.9092915502, -1.9267965512, -1.9337171273; H, 2.277674678, -2.1136269292, -2.5970081082; H, 2.6455671699, -0.7287974634, -1.5464547588.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8540617 (hartree), -2668473.91157847 (kJ mol^{-1}).

TS16b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.3780942 (hartree), -3189449.55744642 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.7067776319, -0.312510014, -0.3823760464; C, -3.4948458506, -0.4539300818, 0.2702665639; C, -2.3689009006, 0.3415254922, -0.0000963133; C, -2.5645309215, 1.3250203298, -0.9840516849; C, -3.7557199408, 1.4987082421, -1.6643943512; C, -4.8363007657, 0.672016025, -1.3600004387; N, -1.2012093688,

0.2815979484, 0.7214750232; C, -0.4079180204, -0.6298319465, 1.0542200483; C, 0.5037432496, -0.8799620343, 1.9897530133; C, 1.4635990264, -1.4929822098, 2.5355609943; O, 2.3672932239, -2.0186117205, 3.0901625139; N, -0.3136198431, -2.0994834417, -0.1859930012; C, -0.7369704263, -1.8344612578, -1.5718791025; C, -0.9036555299, -3.3226009916, 0.3841813133; N, 2.6499990114, -2.5804634627, -0.422019878; C, 3.212868846, -1.7993297522, -1.5329772476; C, 3.0088531844, -4.0005380659, -0.4862766307; N, 1.0383534679, 2.882575606, 1.230475709; C, 1.6989337073, 2.8569285249, 2.5338150917; C, 0.4483147486, 4.1821031905, 0.9196604089; N, 2.8336796992, 1.7833377451, -1.2064973973; C, 4.233579702, 2.1421827009, -1.0197527244; C, 2.2744552179, 2.3282142318, -2.4370296085; F, -1.5161012426, 2.1243778612, -1.2858219874; H, -3.8235042645, 2.2741045827, -2.4168342948; H, -5.7777220414, 0.798116159, -1.879440626; H, -5.5294436676, -0.962550714, -0.1122500195; H, 2.2863692434, 2.116426715, -0.4089365802; H, 4.4229809522, 3.2297867831, -1.0666557721; H, 4.8500051556, 1.6702085943, -1.7934089194; H, 4.582075811, 1.7795301924, -0.049524706; H, 2.7479244994, 1.857813717, -3.30660435; H, 2.4098468936, 3.4201126753, -2.5398399624; H, 1.2034803496, 2.1162948215, -2.4809451154; H, 0.3146678018, 2.1690183108, 1.2045351453; H, 1.0460492221, 3.1816612588, 3.3613257465; H, 2.5699610507, 3.5200764488, 2.5178284177; H, 2.0437832342, 1.844276396, 2.7497037996; H, 1.2408272411, 4.9291328903, 0.8080437181; H, -0.2451734348, 4.54589279, 1.6970580646; H, -0.0957882365, 4.1218726537, -0.0249031352; H, 0.7206230213, -2.2152084258, -0.1975163663; H, -0.3565814309, -2.6171832691, -2.2384397927; H, -1.8234079134, -1.8123903899, -1.6419480142; H, -0.3354083925, -0.8739747518, -1.8948681337; H, -0.6288834157, -4.1984574912, -0.2136791218; H, -0.5298508405, -3.4547557852, 1.3994748861; H, -1.988843647, -3.2325697152, 0.4163427763; H, 3.0009339165, -2.2002661642, 0.4526706711; H, 4.0945143821, -4.1670997324, -0.5565316024; H, 2.6391701994, -4.5167614516, 0.4022472574; H, 2.5451462112, -4.4565900979, -1.3662146248; H, 4.301786174, -1.9294460041, -1.6302856965; H, 2.7559638733, -2.1260209282, -2.4724519612; H, 2.9966069242, -0.7365678548, -1.3901048717; F, -3.3771478237, -1.4045838075, 1.2299364506.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.3865079 (hartree), -3189471.63705429 (kJ mol^{-1}).

TS16c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8947437 (hartree), -2710568.58676653 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.7195977155, -0.8366546911, -0.0972896004; N, -3.4600220303, -0.7944846394, 0.3506916057; C, -2.7493399337, 0.3234438509, 0.1234605418; C, -3.289723768, 1.4291109751, -0.5618623032; C, -4.5921595762, 1.3577469053, -1.0251867713; C, -5.3362445397, 0.1994527274, -0.7897517672; N, -1.4731104877, 0.4337407763, 0.6307712925; C, -0.6066358709, -0.386845131, 0.9991332386; C, 0.4074231623, -0.5308369978, 1.8351057741; C, 1.4433382073, -1.0587627833, 2.3313472134; O, 2.4174125748, -1.501163711, 2.8335945248; N, -0.5615699253, -2.0607183523, -0.1294025868; C, -1.0288501576, -1.9332007579, -1.5161985231; C, -1.152896048, -3.1973932546, 0.5920651899; N, 2.4468334914, -2.6513691164, -0.4383532454; C, 2.9955904416, -1.8956185211, -1.5714134478; C, 2.7205183282, -4.087326239, -0.5276460349; N, 0.7084806537, 3.1040994122, 0.7826691018; C, 1.2976101707, 3.3302596719, 2.1013476554; C, 0.061949122, 4.2958316424, 0.241736307; N, 2.8812860892, 1.7561425598, -1.2189990834; C, 4.2155939149, 1.9581638983, -0.6688130641; C, 2.727710601, 2.333202681, -2.5473455392; H, -2.6800773225, 2.3113336492, -0.7082770059; H, -5.0278237836, 2.1960732416, -1.557412409; H, -6.3615102797, 0.104550333, -1.1248498806; H, -5.2637387179, -1.7536171447, 0.114418365; H, 2.187252844, 2.1613974142, -0.5874891826; H, 4.5328769727, 3.0164969989, -0.6485264129; H, 4.9537395981, 1.4073955925, -1.2626063895; H, 4.2559933643, 1.5726237716, 0.3526780565; H, 3.3716803364, 1.8080624847, -3.2617301154; H, 2.9852319278, 3.4068092691, -2.6000065904; H, 1.6943692096, 2.2161814269, -2.8840711915; H, 0.030739059, 2.3485303586, 0.8435116463; H, 0.5820728242, 3.7352045013, 2.8363272072; H, 2.1265323648,

4.040204895, 2.0168657635; H, 1.6911140819, 2.3899115227, 2.4909038421; H, 0.8116646026, 5.0730290718, 0.0628810891; H, -0.7073023563, 4.7221252036, 0.9082379871; H, -0.4057147754, 4.0608875907, -0.71787931; H, 0.4648590773, -2.1831569281, -0.1540988518; H, -0.6903705407, -2.7856597757, -2.1187532304; H, -2.1159422075, -1.893811488, -1.5431612717; H, -0.6251544363, -1.0178236447, -1.9515206454; H, -0.9413693113, -4.1434836843, 0.0781545282; H, -0.7258895328, -3.2411451403, 1.5949255534; H, -2.2288078631, -3.0487977064, 0.6716890869; H, 2.8559530928, -2.2963070425, 0.4213084927; H, 3.7906395138, -4.3179552008, -0.6487716293; H, 2.3602284413, -4.5900992194, 0.3726684391; H, 2.1911745205, -4.5087816964, -1.3876446262; H, 4.0713633893, -2.0787376107, -1.7228861599; H, 2.4784120784, -2.1932139827, -2.4892405919; H, 2.839500662, -0.8242357131, -1.4181735666.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9017324 (hartree), -2710586.92682567 (kJ mol^{-1}).

TS16d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8847722 (hartree), -2710542.41911022 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.8514042886, -0.8546443429, 0.0495529989; C, -3.6072120071, -0.8298365842, 0.67017973; C, -2.6479082236, 0.0951059859, 0.2329907653; C, -3.0316843312, 0.9820279546, -0.7907663883; N, -4.2187929337, 0.9553806912, -1.3901895691; C, -5.1122557057, 0.0474365307, -0.9794624293; N, -1.4116400745, 0.2336771949, 0.8401292768; C, -0.468638358, -0.5572328292, 1.0826944939; C, 0.5763438681, -0.6384350294, 1.9132930192; C, 1.6762076011, -1.1001263425, 2.3257391329; O, 2.7117934698, -1.4841292659, 2.7564595137; N, -0.3485185015, -2.0395059532, -0.0730279713; C, -0.8658356791, -1.8648202174, -1.4443805326; C, -0.8146689527, -3.2804742278, 0.572849108; N, 2.590238618, -

2.3683873973, -0.5828793125; C, 2.9622090361, -1.5919249864, -1.7745279274; C, 3.0421653997, -3.7618261781, -0.6494591612; N, 0.4756457385, 3.0624172922, 1.0233699823; C, 1.2682591602, 3.2092170189, 2.2433060083; C, -0.3074617268, 4.2561496376, 0.7147419438; N, 2.3487881921, 1.9790867274, -1.3799301407; C, 3.7352696843, 2.2951099697, -1.0583579514; C, 1.9167848264, 2.5761407448, -2.6374249847; H, -2.323832497, 1.7331808992, -1.1297345216; H, -6.0730678877, 0.0523808213, -1.4847049472; H, -5.6144637627, -1.5562456206, 0.3672729057; H, -3.3796388671, -1.4934782238, 1.4964579149; H, 1.7439617257, 2.3061600312, -0.6225737734; H, 3.9530325561, 3.3780762966, -1.0514274286; H, 4.4061915587, 1.8320685246, -1.7907849974; H, 3.9868470062, 1.8925741756, -0.0742495488; H, 2.4673707189, 2.1310738989, -3.4738481899; H, 2.0703107764, 3.6690902113, -2.6868689217; H, 0.8537260456, 2.377573194, -2.7964066988; H, -0.1471001181, 2.2644110081, 1.1231252889; H, 0.6696072129, 3.5122670745, 3.1184820141; H, 2.0424118714, 3.9681663154, 2.0907954117; H, 1.7573343089, 2.2622196007, 2.4769944841; H, 0.3650818953, 5.0877518639, 0.4817358785; H, -0.9625278329, 4.5779176648, 1.5417802442; H, -0.9310832341, 4.0760063068, -0.164168273; H, 0.6892875355, -2.0953997931, -0.1511355882; H, -0.4725718126, -2.6559517805, -2.0922882469; H, -1.9530200774, -1.9062176023, -1.4521621999; H, -0.5394236615, -0.8992465254, -1.8292849994; H, -0.4625044543, -4.1579807248, 0.0202346882; H, -0.4216831038, -3.3206596116, 1.5889206199; H, -1.9042000985, -3.2962901916, 0.603643856; H, 3.0124845222, -1.9347976695, 0.233837035; H, 4.1218094833, -3.8548558329, -0.84130541; H, 2.8163801326, -4.2696090482, 0.290709367; H, 2.5155278452, -4.2811051214, -1.4558551742; H, 4.0410957136, -1.6370058997, -1.987717036; H, 2.4359556059, -1.9930028285, -2.6464105619; H, 2.6712840443, -0.5459197983, -1.6428521118.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8953777 (hartree), -2710570.25053769 (kJ mol^{-1}).

TS16e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8875988 (hartree), -2710549.83680037 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.9194072235, -0.5895968049, 0.1068286025; C, -3.6450861923, -0.616263003, 0.6625680128; C, -2.669890784, 0.2711838389, 0.1746780278; C, -3.0691531346, 1.1637685752, -0.8323474067; C, -4.3689165648, 1.0958934493, -1.3176057042; N, -5.2961626782, 0.2367945053, -0.8749620302; N, -1.4047885631, 0.3493375393, 0.7172515984; C, -0.5284020109, -0.4918842085, 1.0261559764; C, 0.5009501576, -0.6164800891, 1.8639681162; C, 1.5639759696, -1.1387798716, 2.3034497892; O, 2.5653702654, -1.5773261542, 2.7576591214; N, -0.5048885229, -2.0474693845, -0.0830435921; C, -1.049788224, -1.9005537679, -1.4454721229; C, -1.0127085056, -3.2365892492, 0.6238473243; N, 2.4216593218, -2.5428106824, -0.5820511109; C, 2.8693938227, -1.7633557301, -1.7456189671; C, 2.7604867709, -3.9655917637, -0.6897922046; N, 0.6410805466, 3.0729031571, 0.9066284594; C, 1.3211192519, 3.2360777057, 2.1906932931; C, -0.0396139739, 4.2892502815, 0.4714059112; N, 2.6888842029, 1.8275634528, -1.2684747327; C, 4.0476811831, 1.9900141543, -0.7654021744; C, 2.4855754948, 2.4837587078, -2.5534673096; H, -2.3656657458, 1.8866078893, -1.2269814502; H, -4.685252676, 1.7725940583, -2.1067822085; H, -5.6820620862, -1.2702514334, 0.4766015166; H, -3.41487918, -1.2882748489, 1.4804314016; H, 2.0278779221, 2.2038624955, -0.5848985112; H, 4.3732560392, 3.043517886, -0.6986660857; H, 4.7556385643, 1.4705994151, -1.4210447139; H, 4.1284564181, 1.547012484, 0.2300698477; H, 3.0937298214, 1.9972450579, -3.3243375141; H, 2.7513617161, 3.5561985712, -2.5529323292; H, 1.4378790188, 2.3954948368, -2.8525835454; H, -0.031576024, 2.3133543485, 0.9779855986; H, 0.6596890314, 3.6082574169, 2.9907411919; H, 2.1458089882, 3.9477860864, 2.0824088761; H, 1.7349438046, 2.2776474223, 2.5084326665; H, 0.6979609493, 5.0735109469, 0.2737605107; H, -0.7556381446, 4.6831245338, 1.2123043843; H, -0.5802847364, 4.100163085, -0.4592727241; H, 0.527046062, -2.1519626709, -0.1769191053; H, -0.7181595841, -

2.7353113102, -2.0733114481; H, -2.1376640976, -1.8846267567, -1.4218846702; H, -0.6868398006, -0.9687465739, -1.8782839386; H, -0.7135038323, -4.1528618685, 0.1035217229; H, -0.6008472357, -3.2530692528, 1.6331922068; H, -2.1009148734, -3.200309227, 0.6766745802; H, 2.8695214988, -2.1696272217, 0.2507031938; H, 3.8312802691, -4.1393680217, -0.874871342; H, 2.4827199499, -4.4839508359, 0.2305887938; H, 2.203379962, -4.4142371751, -1.5177529723; H, 3.9405605079, -1.9017361767, -1.9582007381; H, 2.3128611978, -2.0839575367, -2.6319233173; H, 2.6785678006, -0.6994198524, -1.5788179757.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.8979737 (hartree), -2710577.06307701 (kJ mol^{-1}).

Int6a

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8675115 (hartree), -2668509.20714522 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.9230452169, -2.1651757665, -0.2639205573; C, -4.0165837417, -2.0538137986, 0.7895312576; C, -2.6613815999, -1.8396059617, 0.5488679455; C, -2.183038959, -1.7379897158, -0.7714494092; C, -3.1061544448, -1.8663872325, -1.8259864822; C, -4.4577908462, -2.069617798, -1.576509165; N, -0.8475787956, -1.5514659416, -1.1461692936; C, 0.094913216, -1.1884681675, -0.3543235204; N, 1.4422348144, -1.1162509783, -1.1381220307; C, 1.7371913287, -2.3953823654, -1.8405301774; C, 0.2055852526, -0.8240639266, 0.9694643991; C, 0.9564642745, -0.4559002586, 1.9141335916; N, 0.9751058489, 3.1572544822, -0.5937547419; C, 0.5718048091, 4.085573308, -1.6437704323; C, 1.4474735941, 0.0485011177, -2.0748710879; O, 1.6007107972, -0.1008214132, 2.8552544771; C, 2.0080517374, 3.7101174552, 0.275133745; N, 3.8094665769, -0.7549660752, 0.615952093; C, 4.3859052326, -2.0434739429, 1.0190372758; C, 4.8105619164, 0.1572551871, 0.0512676511; N, -1.5234336268,

2.241213206, 1.1574841941; C, -2.8222950782, 2.3627313142, 0.4977614936; C, -1.5325896567, 2.7593757789, 2.5244742241; H, -2.732864618, -1.8022457191, -2.8417662818; H, -5.1497415184, -2.1600474557, -2.4069783682; H, -5.9763301174, -2.3290105339, -0.0659044062; H, -4.3660515473, -2.1346721444, 1.8135442559; H, -1.9681853089, -1.752843045, 1.3743219955; H, 0.157843814, 2.9076245963, -0.0285609417; H, 1.73753172, 4.6847341011, 0.7181718267; H, 2.936593973, 3.8559070012, -0.2889237036; H, 2.2137762195, 3.0146042721, 1.0924322549; H, 1.4058418526, 4.2601002241, -2.3328234357; H, 0.2471917216, 5.0699779299, -1.2630927132; H, -0.2529392329, 3.6575121654, -2.2192141787; H, -1.2428423435, 1.2628281117, 1.1743777946; H, -2.3240217373, 2.3185689045, 3.1531844408; H, -1.6873055632, 3.8430555463, 2.5069336945; H, -0.5695822549, 2.561793736, 2.9997341262; H, -3.0636458599, 3.4208837798, 0.353862917; H, -3.6465291127, 1.9033869535, 1.0670714128; H, -2.7840916844, 1.8867598163, -0.4842732345; H, 2.2093212814, -0.9621512379, -0.4378307031; H, 2.411578657, 0.0799328186, -2.5860797966; H, 0.6425339933, -0.0930488864, -2.7938027456; H, 1.2961231829, 0.9723309454, -1.5084622529; H, 2.7068610621, -2.3110317215, -2.3333562889; H, 1.7610681777, -3.2002049982, -1.1066932851; H, 0.9474470857, -2.5846751169, -2.5630479424; H, 3.3968019508, -0.3221446231, 1.440249311; H, 5.2312516796, -1.9344864338, 1.7139396926; H, 3.6192244292, -2.6506490625, 1.504012843; H, 4.7445153165, -2.5804719855, 0.1358691324; H, 5.663097256, 0.326836843, 0.7254054554; H, 5.2015678466, -0.2561508306, -0.8832509175; H, 4.3472786699, 1.1210231418, -0.1686818303.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8764134 (hartree), -2668532.56790938 (kJ mol^{-1}).

Int6b

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.3991433 (hartree), -3189504.79543614 (kJ mol^{-1}). Structure definition (3D

Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.5347081705, 0.5415517528, -0.5220441612; C, -5.093040032, -0.2557904244, 0.4748366487; C, -4.3777012293, -1.3353957457, 0.9884927164; C, -3.1083659077, -1.592969979, 0.4993725665; C, -2.4939756746, -0.8209648435, -0.4966773448; C, -3.2639116636, 0.2423337059, -0.9831930761; N, -1.2588705722, -1.1361663107, -1.0611579078; C, -0.1900193373, -1.0609343089, -0.3489295696; C, 0.0876915313, -0.6219165088, 0.9230611294; C, 0.9800733912, -0.4597666811, 1.8014759326; O, 1.7647706144, -0.268363142, 2.6792159131; N, 1.0326157825, -1.5301615022, -1.1654882372; C, 1.4372066839, -0.4795000665, -2.1528986648; C, 0.7937548746, -2.8478668063, -1.8202891831; N, 3.3827199062, -2.0291817375, 0.5260947952; C, 4.6577542494, -1.7527572014, -0.1466305427; C, 3.3342686685, -3.3762383318, 1.1104800171; N, 2.387885625, 2.5639004209, -0.8027467226; C, 3.574409836, 2.6397061355, 0.0423441964; C, 2.4239770929, 3.5162593144, -1.9068400632; N, -0.1930043635, 2.9014737489, 1.0267354219; C, 0.0964669288, 3.3586126721, 2.3853183742; C, -1.3137999602, 3.6131849994, 0.4157832124; F, -2.7222873342, 1.0229481434, -1.9513400351; H, -5.0639222625, 1.3874694926, -0.9420449813; H, -6.0855746201, -0.0377895581, 0.8490232636; H, -4.7859587732, -1.9779148802, 1.7583176683; F, -2.4345268116, -2.6660618327, 0.9759984986; H, 1.5561858449, 2.735388725, -0.2295486853; H, 3.7821773548, 3.6558961408, 0.4210433762; H, 4.4586073925, 2.3153195384, -0.5188149679; H, 3.4563642706, 1.977063175, 0.9030331321; H, 3.2357196848, 3.2613422863, -2.5975561233; H, 2.5814633892, 4.5608059472, -1.5850884669; H, 1.4848662724, 3.4724562212, -2.4642792133; H, -0.3937839813, 1.9039052991, 1.0478607635; H, -0.7827020768, 3.3324206069, 3.0503211158; H, 0.4611104365, 4.3905532189, 2.3565014737; H, 0.876148602, 2.7339265714, 2.8253481569; H, -1.0435476994, 4.663224698, 0.2638838721; H, -2.2314060825, 3.5893261719, 1.0269616822; H, -1.5411277154, 3.1773276997, -0.5592294151; H, 1.8340941093, -1.6573557954, -0.4931465369; H, 2.306585056, -0.8412580169, -2.7045128015; H, 0.6015951624, -0.3110438636, -2.8299643607; H, 1.6929037457, 0.4411067107, -1.6193633594; H, 1.7134631481, -3.1592443544, -2.3173349312; H, 0.5158792467, -3.572962589, -1.0566534561; H, -0.0189524782, -2.7438227936, -2.5342626556; H, 3.2545614627, -1.355702339, 1.2790875546; H, 4.1726232595, -

3.5734886228, 1.7936851688; H, 2.4021603601, -3.5001282784, 1.6646022527; H, 3.3660541738, -4.1254978697, 0.3140268983; H, 5.5276444099, -1.90577929, 0.5085275222; H, 4.7701504618, -2.4145233841, -1.0104913756; H, 4.6698679094, -0.7204309584, -0.5016206235.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1215.4094697 (hartree), -3189531.89443691 (kJ mol^{-1}).

Int6c

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9117225 (hartree), -2710613.14329294 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.7077959832, -0.7491772667, -1.082449313; C, -5.2004016285, -0.9423054014, 0.2060475162; C, -4.2896685416, -1.2963231176, 1.1998634377; C, -2.9474200112, -1.4315790104, 0.8750376516; C, -2.5455415578, -1.2202037896, -0.4585431512; N, -3.4258342908, -0.8916610186, -1.420610184; N, -1.2385372337, -1.390781298, -0.9106480236; C, -0.1958306443, -1.2098295107, -0.1848105039; C, 0.0584462212, -0.7668312777, 1.0931997416; C, 0.927211052, -0.5281755041, 1.9779923666; O, 1.6854776821, -0.2772424217, 2.8640705618; N, 1.0788741167, -1.5451505082, -1.0140882989; C, 1.2775784889, -0.5403418865, -2.1044671664; C, 1.0251595271, -2.9355053158, -1.5465389865; N, 3.5839078763, -1.5160977223, 0.5788020088; C, 4.6703896913, -0.8087877971, -0.1093408531; C, 3.9760013032, -2.862323976, 1.0132183385; N, 1.577924727, 2.7574683078, -1.0652256619; C, 2.7287827861, 3.2382018016, -0.3096378221; C, 1.3078131175, 3.5654459475, -2.2490608131; N, -0.9524009845, 2.5924673302, 0.8625750786; C, -0.7722531816, 3.3033644404, 2.1268333113; C, -2.2369565959, 2.8829811277, 0.2275641947; H, -5.3811457367, -0.4723416069, -1.8900987182; H, -6.2562287033, -0.823110092, 0.4174034677; H, -4.6203285958, -1.4628757502, 2.2196290095; H, -2.2130040593, -1.6898971172, 1.6253018028; H, 0.7525662279, 2.7543484654, -0.4583301484; H, 2.6609254404,

4.3045979442, -0.0307744494; H, 3.6448509175, 3.1139371955, -0.8986606778; H, 2.8364128906, 2.6564327717, 0.6092026097; H, 2.1309367362, 3.4695905877, -2.9660740691; H, 1.1840592146, 4.6408545828, -2.0311992036; H, 0.3962240196, 3.2122554426, -2.7374741465; H, -0.8747601014, 1.5910201101, 1.0288112769; H, -1.5955117892, 3.1391792687, 2.841903482; H, -0.7057987311, 4.3796972031, 1.9379686861; H, 0.1589375573, 2.9847893971, 2.6000882448; H, -2.2628882128, 3.9316723787, -0.085844666; H, -3.1004969649, 2.7097481396, 0.8904834036; H, -2.3601758683, 2.2602418852, -0.6607898475; H, 1.907364262, -1.485963252, -0.3718930465; H, 2.1801035875, -0.8055795128, -2.6581541328; H, 0.405764769, -0.574005981, -2.7550312526; H, 1.3886636236, 0.4549437799, -1.6641557136; H, 1.9505724049, -3.1412569966, -2.0860158634; H, 0.9197762261, -3.6270933644, -0.7112374624; H, 0.1635662928, -3.0200296633, -2.2044279315; H, 3.3145370622, -0.9824515188, 1.4031591906; H, 4.8850440552, -2.8638313088, 1.6321583362; H, 3.1663173057, -3.3105461248, 1.5923671112; H, 4.1644492182, -3.4924098667, 0.1389499935; H, 5.590599752, -0.7525678606, 0.4905852546; H, 4.9120095571, -1.3236941317, -1.043928089; H, 4.3522124491, 0.2069119518, -0.3515690716.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9234408 (hartree), -2710643.89497994 (kJ mol^{-1}).

Int6d

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9092523 (hartree), -2710606.66088361 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, -4.9443942599, -1.5395408609, 0.1029283504; C, -4.9456073673, -1.5031396031, 1.4421203305; C, -3.7775933005, -1.447736384, 2.1973855707; C, -2.5454789682, -1.4188464274, 1.5511687308; C, -2.5200155887, -1.4511716177, 0.1467496014; C, -3.7652390924, -1.5199806153, -0.510786567; N, -1.3941507985, -

1.4533595648, -0.6760622229; C, -0.1988573488, -1.2015237257, -0.2764737043; C, 0.3930350251, -0.8300020207, 0.9096667774; C, 1.4622544966, -0.5467182095, 1.5193275203; O, 2.42461252, -0.2625513137, 2.1644480398; N, 0.7928137379, -1.3244946045, -1.4693139876; C, 0.6192274475, -0.1854693576, -2.4228865561; C, 0.6704252701, -2.642983149, -2.1515721896; N, 3.6353131236, -1.2611901324, -0.6509784041; C, 4.4811646369, -0.5312978055, -1.6030865861; C, 4.1450813964, -2.6079216699, -0.3630114334; N, 1.1380707707, 2.9794507931, -1.0957035999; C, 2.4712915701, 3.3973850942, -0.676317987; C, 0.5252428483, 3.9189081158, -2.0284686985; N, -0.7077413378, 2.4999733943, 1.4556000521; C, -0.1894156997, 3.0236306619, 2.7185350079; C, -2.1198340051, 2.8168147192, 1.2483509719; H, -3.7720565172, -1.5584362543, -1.5969690282; H, -5.9188953041, -1.5231541401, 1.9238120705; H, -3.8312043424, -1.4283620638, 3.2803657117; H, -1.620700517, -1.374806405, 2.1104477541; H, 0.5406446149, 2.8821783486, -0.2693354437; H, 2.5028084769, 4.4187691082, -0.2581999634; H, 3.1593279848, 3.373953368, -1.5292613343; H, 2.8509787227, 2.7106991714, 0.0842010329; H, 1.0863316337, 3.9350036144, -2.9695403375; H, 0.4860543493, 4.9554296574, -1.6502645449; H, -0.4964665397, 3.6031833373, -2.2542493239; H, -0.5803650282, 1.4904233063, 1.436348045; H, -0.7823049623, 2.7148976383, 3.595453289; H, -0.1849198632, 4.1178840461, 2.6892368838; H, 0.8380156072, 2.6839047268, 2.8640866368; H, -2.2404856678, 3.898876945, 1.1354708065; H, -2.7682324819, 2.4910789547, 2.077876548; H, -2.4756964944, 2.3400773157, 0.3325421175; H, 1.7679315599, -1.2653394531, -1.0812176281; H, 1.340074354, -0.2996778258, -3.2345621363; H, -0.396657047, -0.2222072566, -2.8119662843; H, 0.7969702385, 0.7586053201, -1.8989808674; H, 1.4182025335, -2.6986255373, -2.943839044; H, 0.8424192942, -3.4325671187, -1.4210082425; H, -0.3340672951, -2.7335818588, -2.5566868318; H, 3.6019011281, -0.7429014081, 0.2247726351; H, 5.1886188255, -2.6039399127, -0.0166691387; H, 3.5291630984, -3.0744343677, 0.4080624973; H, 4.0933166214, -3.2232959686, -1.2659989662; H, 5.5311214975, -0.4694946644, -1.2816233137; H, 4.4589832329, -1.0323765638, -2.5753536305; H, 4.0988215548, 0.4830852404, -1.732030337.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9204511 (hartree), -2710636.04927548 (kJ mol^{-1}).

Int6e

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9104567 (hartree), -2710609.82152396 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -4.9149535137, -1.31995991, 0.2376958327; N, -4.933470565, -1.4623409401, 1.5694188617; C, -3.7439811209, -1.5900869204, 2.1677226173; C, -2.5193624612, -1.5711704059, 1.5064417211; C, -2.5054205971, -1.4195886236, 0.1084208121; C, -3.7548451257, -1.3013025203, -0.5243046752; N, -1.378076739, -1.4234452787, -0.7106431442; C, -0.1826235067, -1.189946037, -0.2934682839; C, 0.3956727034, -0.8181553483, 0.8957500536; C, 1.4594846329, -0.541408155, 1.5182447137; O, 2.4155053491, -0.2645947137, 2.1742137964; N, 0.8216112865, -1.3349607126, -1.4720257393; C, 0.6677982702, -0.2068546078, -2.4421948943; C, 0.6959700864, -2.6615229121, -2.1382964671; N, 3.6539851277, -1.2872912615, -0.6199588982; C, 4.5141268271, -0.5422002541, -1.5474239217; C, 4.1586999089, -2.6394251954, -0.3481539726; N, 1.0941310465, 2.9533031178, -1.1047499734; C, 2.4216527498, 3.3816742763, -0.6775279989; C, 0.4773290516, 3.8914220768, -2.0362260073; N, -0.7597025008, 2.4827232088, 1.4450382745; C, -0.2280402965, 3.0321248998, 2.6917180582; C, -2.1722727878, 2.8032773399, 1.2438294862; H, -3.798353478, -1.1976854047, -1.6020685838; H, -5.8835536678, -1.2212553675, -0.2454881362; H, -3.766670573, -1.713275519, 3.2475827339; H, -1.5976575393, -1.6742402283, 2.0616817448; H, 0.493219307, 2.8477565462, -0.2815871974; H, 2.4416989954, 4.4009220763, -0.2537311605; H, 3.1131570253, 3.3694600235, -1.5279479893; H, 2.8050352504, 2.694571318, 0.080790772; H, 1.0423268227, 3.916426511, -2.9748075261; H, 0.4276919772, 4.9257937174, -1.6536205938; H, -0.5406728099, 3.567813036, -2.2674587016; H, -0.6403127742, 1.4720665088, 1.4495953209; H, -0.8152089842, 2.7466057001, 3.5799807058; H, -0.2180059827,

4.1253933409, 2.6371493273; H, 0.798936747, 2.6905326217, 2.8365866211; H, -2.2872830725, 3.8829074433, 1.1044204958; H, -2.8137135175, 2.5027608994, 2.0877728469; H, -2.5400011468, 2.3051392319, 0.3442432554; H, 1.7930334191, -1.2786091032, -1.0734727715; H, 1.4068605176, -0.3300630064, -3.2359349239; H, -0.3392109111, -0.2493454304, -2.8528704644; H, 0.8306002547, 0.7436317057, -1.9244176584; H, 1.4519908558, -2.733370984, -2.9212743886; H, 0.8535518052, -3.4429518102, -1.3957722322; H, -0.3046196178, -2.7490485244, -2.5537941529; H, 3.6105337484, -0.7834496285, 0.2638219737; H, 5.1963013338, -2.6422097024, 0.0153737564; H, 3.5301485931, -3.1199172043, 0.4039982512; H, 4.1218002462, -3.23815281, -1.2629391484; H, 5.5597730919, -0.489435788, -1.2109146147; H, 4.5035490616, -1.0247231246, -2.5292478784; H, 4.1362597162, 0.4755275111, -1.6622781642.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1032.9221851 (hartree), -2710640.59971584 (kJ mol^{-1}).

TS26a

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8770452 (hartree), -2668534.22590719 (kJ mol^{-1}). Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8660962 (hartree), -2668505.49305166 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -3.373872934, -0.6336256373, -1.5998925952; C, -4.5470235322, 0.1119813129, -1.6249661729; C, -5.0431445747, 0.6833179548, -0.4521378729; C, -4.3470218912, 0.4969886212, 0.7418624208; C, -3.1616000138, -0.2340918611, 0.7717970668; C, -2.6500991847, -0.8099227963, -0.4063184815; N, -1.5076185997, -1.6151218567, -0.4757168533; C, -0.488093649, -1.4812288002, 0.3037591415; N, 0.597316069, -2.5042015072, 0.0377844743; C, 0.7712208386, -3.4047284401,

1.2059509803; C, -0.1664489159, -0.5619570645, 1.291354483; C, 0.6249188323, -0.0849049372, 2.1447892083; O, 1.323956543, 0.4477776949, 2.960288001; C, 0.3877895421, -3.3013351505, -1.1929425236; N, 2.8253191415, -1.1571584839, -0.2868381983; C, 3.6960809312, -1.3098827779, 0.8988717026; C, 3.4900844503, -1.5900134267, -1.5306286928; N, -0.4179248938, 2.6201874803, 0.0302907305; C, -1.3005615045, 2.9997191195, -1.071990264; C, -0.4636854869, 3.5700398182, 1.1423205628; N, 2.518769887, 1.7802290026, -0.6072118219; C, 2.8718621033, 2.2599001337, -1.9447319023; C, 3.3305284742, 2.4124860872, 0.4390011966; H, -2.9940788736, -1.0993691833, -2.5024323719; H, -5.0822599972, 0.2392582312, -2.5600811573; H, -5.9631056252, 1.2569019243, -0.4674001577; H, -4.7297126781, 0.9244455302, 1.6629560195; H, -2.6297623795, -0.3691802935, 1.7037355686; H, 1.5338804758, 2.0205924403, -0.4292954422; H, 3.2896690033, 3.512343715, 0.4030311381; H, 4.3801080036, 2.1180671149, 0.3305851656; H, 2.9805068917, 2.0857232523, 1.4199810075; H, 3.8930546611, 1.9560289433, -2.1987740517; H, 2.819885435, 3.3563483867, -2.0367862428; H, 2.1948233615, 1.8260874376, -2.6847814383; H, -0.6822155306, 1.6988333177, 0.3763582863; H, -1.4856811356, 3.7561231298, 1.5106970667; H, -0.0443742001, 4.5308041015, 0.8257613973; H, 0.1359964896, 3.1922905474, 1.9727357692; H, -0.9354728951, 3.9220140134, -1.5360349876; H, -2.3420741712, 3.1681323485, -0.7565395954; H, -1.302182645, 2.2142312041, -1.8305865671; H, 1.692566623, -1.8211724617, -0.1104782903; H, 1.2541732231, -3.9540094178, -1.3270365868; H, -0.5210025004, -3.8994940478, -1.123253938; H, 0.2864353962, -2.6347779376, -2.0464934665; H, 1.6325432952, -4.0544405728, 1.0356881017; H, 0.9339129419, -2.8089195499, 2.1009721511; H, -0.1212526061, -4.0226904492, 1.3410034353; H, 2.5974213268, -0.1399669873, -0.3851186268; H, 4.6410082203, -0.7745263802, 0.7618535273; H, 3.1880428492, -0.9072172182, 1.7748171495; H, 3.9184388921, -2.3671862225, 1.0628900914; H, 4.4218406908, -1.039443327, -1.6957989337; H, 3.7236890794, -2.6562154243, -1.480248244; H, 2.8268938975, -1.4158331034, -2.3789776499.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version =

AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -1016.8675316 (hartree), -2668509.25989254 (kJ mol^{-1}).

TS5-6a

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -611.221483 (hartree), -1603994.75501431 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.0090162466, -0.0396913896, -0.0099115544; C, -0.0157846439, -0.0051369245, 1.3939206865; C, 1.2057006929, 0.0382282639, 2.0824547615; C, 2.4047344194, 0.0745249714, 1.3795925261; C, 2.4089498404, 0.0557052644, -0.015584167; C, 1.1976270108, -0.006211888, -0.703148134; N, -1.1908748809, -0.0520152089, 2.1286686342; C, -2.3576013562, 0.3053626808, 2.0346042896; C, -3.6685239553, 0.24197354, 2.4751863764; C, -4.2799870636, 1.2949724772, 1.7721061627; N, -3.0436585095, 1.7495519772, 0.9726623681; C, -2.5787436201, 3.0952444782, 1.3443582511; O, -5.3590941055, 1.8247764412, 1.6636094297; C, -3.2447439709, 1.6046209367, -0.4777111374; H, -4.0835947662, -0.4469213037, 3.1937799608; H, 1.1931974897, 0.0459213229, 3.1655889369; H, 3.3412461239, 0.1138265027, 1.9245398426; H, 3.345431354, 0.0797299566, -0.5602933297; H, 1.1901986964, -0.0377517185, -1.7872079168; H, -0.94643479, -0.1163235293, -0.545758991; H, -3.5009949458, 0.5690535897, -0.7063981979; H, -2.3327553863, 1.8813388506, -1.0080411339; H, -4.0661836251, 2.24997137, -0.8067905603; H, -1.6231345562, 3.2973961241, 0.8570956975; H, -2.4453502633, 3.1438784104, 2.4254886436; H, -3.3103065567, 3.8509485893, 1.0401700128.

TS5-6b

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -809.7523539 (hartree), -2124988.34651742 (kJ mol^{-1}). Structure definition (3D

Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, 1.5484000532, 1.0898979815, -0.4125037024; C, 1.2913946197, -0.2900248326, -0.3942498793; C, 2.3486516995, -1.0945254632, 0.0606839566; C, 3.561724009, -0.5787007593, 0.4811938329; C, 3.7591579333, 0.8006550685, 0.4496579322; C, 2.7466712425, 1.6453576657, -0.0012474834; N, 0.1258477835, -0.8586908482, -0.8452623223; C, -1.0734788857, -0.5900731176, -0.8501326515; C, -2.3183094898, -0.6922433084, -1.4241762022; C, -3.1687046548, -0.2124204574, -0.4031134841; N, -2.0859121792, 0.1256542815, 0.6274126964; C, -2.1527372576, -0.7096015472, 1.8362389843; O, -4.3449497611, -0.0407265792, -0.2055851802; C, -2.0228702647, 1.5632289249, 0.9315711268; H, -2.5564939854, -1.0512504487, -2.4131240749; F, 2.1567047786, -2.4277023117, 0.0918325238; H, 4.3310550791, -1.2583672634, 0.8244090767; H, 4.7043342654, 1.217729345, 0.7735710809; H, 2.87459417, 2.719324394, -0.0473077082; F, 0.5679960572, 1.9044890959, -0.8694451133; H, -1.8949271432, 2.1246845677, 0.0069925732; H, -1.1748170129, 1.7608540907, 1.5890783088; H, -2.9470035837, 1.8832904641, 1.4244061614; H, -1.2697899319, -0.526472878, 2.4515584811; H, -2.1746252742, -1.7612467557, 1.5486716595; H, -3.0520716611, -0.4767517214, 2.415602128.

TS5-6c

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2636296 (hartree), -1646093.27367121 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.0269658042, -0.1674810169, -0.0238894294; C, 0.0139726777, 0.0196424191, 1.3701426438; N, 1.1582284851, 0.1924459259, 2.0409721723; C, 2.2949136267, 0.2054475516, 1.3421232685; C, 2.3617940097, 0.043110343, -0.0394921641; C, 1.1670245697, -0.1520436695, -0.7301917404; N, -1.141269984, -0.005487155, 2.1297875775; C, -2.3188256518, 0.3082797109, 2.0234522824; C, -3.6345258067, 0.2059940475, 2.429446273; C, -4.2567694851, 1.265461774, 1.7404783768; N, -3.0204488069, 1.7776122538, 0.9848819285; C, -2.5943805667, 3.1191612829, 1.4140080302; O, -5.3483914794,

1.7658227835, 1.6259540925; C, -3.1799658975, 1.6771361839, -0.4740459338; H, -4.0488108869, -0.5097970748, 3.1218412598; H, 3.2019113694, 0.3512714572, 1.9223171994; H, 3.3161735446, 0.0600190083, -0.5508969955; H, 1.1655892539, -0.2986867372, -1.8047369193; H, -0.972377403, -0.341703887, -0.5207578468; H, -3.4281404968, 0.6490206168, -0.7417986601; H, -2.2519786072, 1.9693426568, -0.9673113206; H, -3.9916907508, 2.331534295, -0.8095788234; H, -1.6346326473, 3.3598806734, 0.9528673617; H, -2.480947259, 3.1316602959, 2.49830576; H, -3.3363827262, 3.8694237258, 1.1216864936.

TS5-6d

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2603069 (hartree), -1646084.55409325 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.014000014, -0.0578974999, -0.0368669135; C, -0.0163508392, 0.0097241429, 1.3625838971; C, 1.2283117171, 0.065668594, 2.0146813206; N, 2.395115182, 0.0830982646, 1.3771446312; C, 2.3815505996, 0.0338890502, 0.0400670483; C, 1.2057858772, -0.0411895589, -0.7034056771; N, -1.1672374292, -0.0139013043, 2.1270607748; C, -2.3432755981, 0.3175382078, 2.033732803; C, -3.6500858135, 0.2336808283, 2.471654898; C, -4.2790062846, 1.2830273492, 1.773827438; N, -3.0544268864, 1.7643308577, 0.9760242446; C, -2.6134207635, 3.1160101973, 1.3566718209; O, -5.3673511358, 1.7922551808, 1.672095526; C, -3.2552309089, 1.6252928493, -0.4750557246; H, -4.056240151, -0.4675155461, 3.1835220867; H, 1.2526088849, 0.09972009, 3.0998734887; H, 3.3488897213, 0.0481068784, -0.4524483769; H, 1.2461185383, -0.0953766383, -1.7852609339; H, -0.9470513835, -0.1414868884, -0.5799794413; H, -3.4977472824, 0.5877805662, -0.7101382292; H, -2.3478080181, 1.918705918, -1.0045703992; H, -4.0853840662, 2.2611039834, -0.8005977688; H, -1.6635999981, 3.340159302, 0.8676861917; H, -2.4767789498, 3.1592128979, 2.4375731794; H, -3.3595429067, 3.8604148214, 1.0604300746.

TS5-6e

Optimised geometry: Program version = AM64L-G03RevD.01. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -627.2625937 (hartree), -1646090.55521609 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): C, -0.0015208317, -0.0373017101, 0.0255038481; C, -0.005416784, 0.0185008557, 1.4278737688; C, 1.235917138, 0.0341835255, 2.0781600598; C, 2.3942349313, 0.0156009082, 1.3110911531; N, 2.409136186, -0.024295219, -0.0268350676; C, 1.2207027186, -0.0544225161, -0.6381635111; N, -1.1618569686, 0.0299775062, 2.1793801026; C, -2.3436262345, 0.331776643, 2.0541771541; C, -3.6557164861, 0.2329742936, 2.4614179894; C, -4.2882554808, 1.2712603154, 1.7456489601; N, -3.0635710613, 1.7740552046, 0.970655584; C, -2.6525812969, 3.1330887229, 1.3586099099; O, -5.3851845613, 1.7566448304, 1.6271237767; C, -3.2359942525, 1.6323611183, -0.484097069; H, -4.0663025751, -0.4701137234, 3.1691169479; H, 1.2801566665, 0.0634290608, 3.1595896298; H, 3.3648263941, 0.0329535207, 1.798653476; H, 1.24310712, -0.09935177, -1.7238112041; H, -0.9289986335, -0.088686317, -0.529435058; H, -3.4579146315, 0.5914253045, -0.724047376; H, -2.3228894861, 1.9391198334, -0.9955611784; H, -4.0691112499, 2.2559549217, -0.8252603615; H, -1.696768917, 3.3707466168, 0.8881164471; H, -2.5381978168, 3.1800908212, 2.4419839138; H, -3.4035903362, 3.8658740634, 1.0460495671.

dimethylamine

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -135.2096335 (hartree), -354823.168022397 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, -0.181570041, -0.3615743984, 0.4138228103; H, -0.3281497072, -0.1248103323, 1.3884907896; C, 1.2226782019, -

0.1877374419, 0.0643143099; C, -1.0879939894, 0.4090097696, -0.4281416039; H, -2.1156730417, 0.2751431925, -0.0827312266; H, -0.8668336849, 1.4908281018, -0.4524707495; H, -1.0330194361, 0.0373181461, -1.4560234237; H, 1.4000770975, -0.5909871245, -0.9375028707; H, 1.5578987895, 0.864623382, 0.0643561707; H, 1.8485849946, -0.7487285429, 0.7620854024.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -135.2129612 (hartree), -354831.900721582 (kJ mol^{-1}).

dimethylamine dimer

Optimised geometry: Program version = AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -270.4240884 (hartree), -709658.98857833 (kJ mol^{-1}). Structure definition (3D Coordinates, Atom, X coord/ Angstrom, Y coord/ Angstrom, Z coord/ Angstrom): N, 1.6215479777, 0.2294549868, -0.3234597614; C, 2.3663256601, -0.9927463023, -0.5837365511; C, 2.0969448943, 0.9478740858, 0.8488334739; H, 0.6278669359, 0.0214396357, -0.230564853; H, 2.3961003395, -1.6918164224, 0.2730751138; H, 3.4025220463, -0.7503186021, -0.8435475902; H, 1.9276740905, -1.5183370352, -1.4358696251; H, 3.1174517476, 1.3075746051, 0.6778147606; H, 2.1121240247, 0.3394155231, 1.7724228421; H, 1.4655464858, 1.8218530261, 1.0278743873; N, -1.5980301734, -0.2854788845, -0.2975099336; C, -2.2644390089, -0.8769219304, 0.8607708676; C, -2.1179970878, 1.0352665745, -0.6484955146; H, -1.6902739984, -0.9063404403, -1.0948595335; H, -3.3601666758, -0.9423832831, 0.7549068106; H, -2.0513289441, -0.2740890083, 1.7483086162; H, -1.8735136159, -1.8811880992, 1.0384710773; H, -1.9085241677, 1.7346073324, 0.1661058331; H, -3.2054582393, 1.0468940762, -0.8300297324; H, -1.6096514058, 1.4040214101, -1.5415538965.

Solvent field (PCM model) calculation with ether. Single-point energy calculation: Program version =

AM64L-G03RevC.02. RB3LYP/6-311++G(d,p). Calculated Energy E(HF) = -270.4280679 (hartree), -709669.431760229 (kJ mol^{-1}).