

Effect of the tether length upon Truce-Smiles rearrangement reactions

David Fuss, Yu Qi Wu, Michael R. Grossi, Joshua W. Hollett, Tabitha E. Wood*

Department of Chemistry, The University of Winnipeg, 515 Portage Avenue, Winnipeg, Manitoba, Canada, R3B 2E9

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Table S1: Free energies of reaction for formation of Meisenheimer adduct intermediate, relevant bond angles, and LMO-EDA energy of interaction for the intermediate. The energies are given in kJ mol^{-1} .

n	$\Delta G(\text{sol})$	$\Delta G(\text{gas})$	$\angle \text{CCN-C}_{\text{spiro-O}} (\text{sol})$	$\angle \text{CCN-C}_{\text{spiro-O}} (\text{gas})$	$E_{\text{int}}[\mathbf{1-2}]^{\text{a}}$
2	-51.0	-53.2	101.4°	99.5°	-709
3	-36.1	-38.6	108.4°	106.9°	-661

^aLMO-EDA energy calculated from two separate energy decomposition calculations (in the gas phase). A calculation with 3 fragments (1, 2, and 3) yielded $E_{\text{int}}[\mathbf{1-2-3}]$ and a calculation with only 2 fragments (fragments 1 and 2 were combined) yielded $E_{\text{int}}[\mathbf{12-3}]$. The interaction energy between the fragments of interest (1 and 2) is obtained by subtraction, $E_{\text{int}}[\mathbf{1-2}] = E_{\text{int}}[\mathbf{1-2-3}] - E_{\text{int}}[\mathbf{12-3}]$. (See Figure S1)

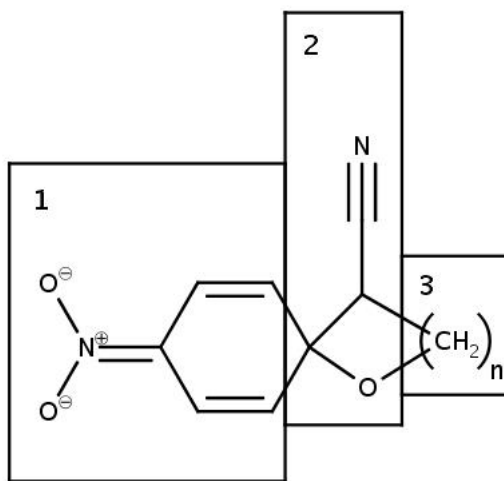


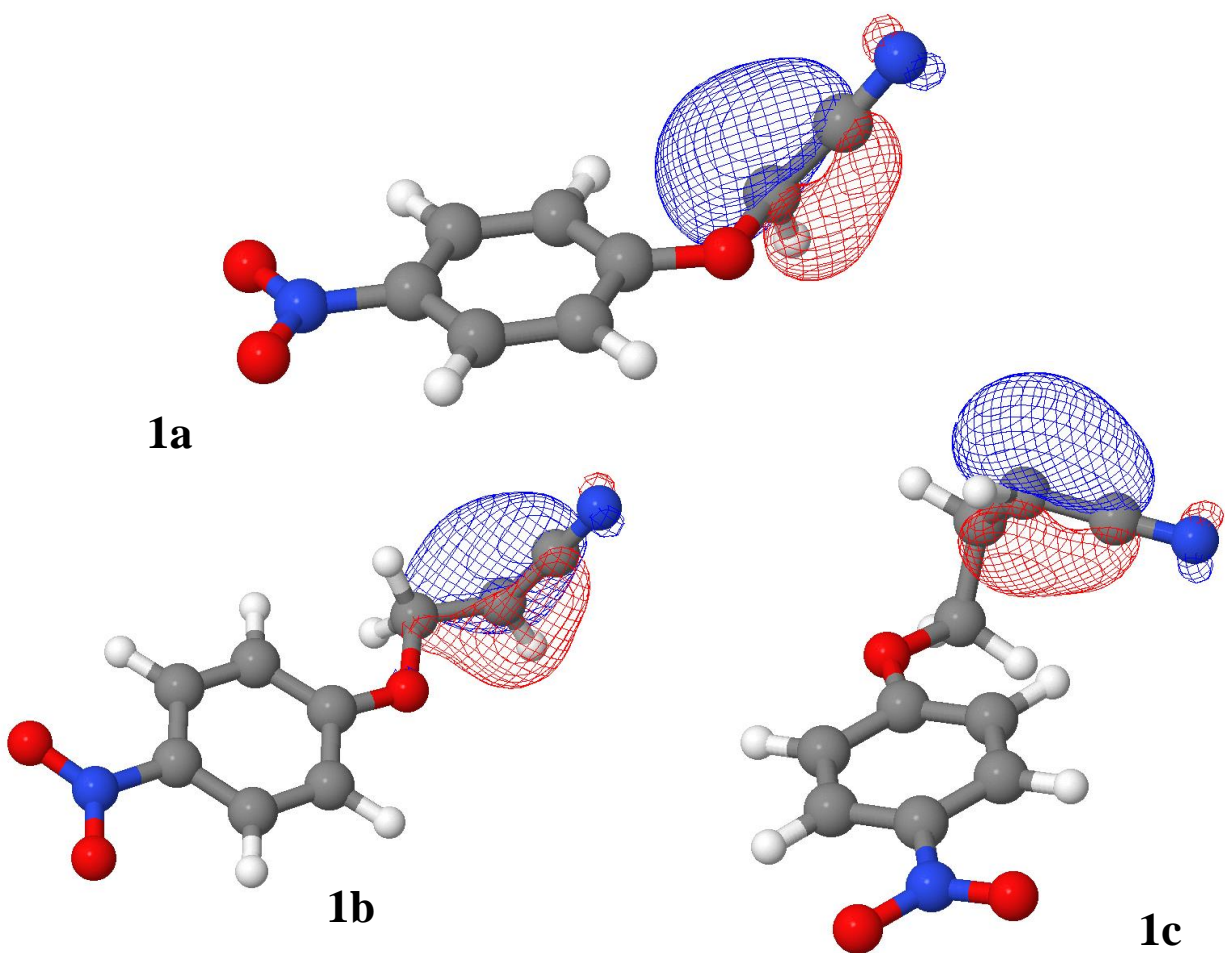
Figure S1: Fragmentation scheme for determination of LMO-EDA interaction energies.

Table S2: Mayer^[1] bond order between oxygen and non-phenyl carbon of reactant (**1a**, **1b**, **1c**)
[ω B97X-D/6-31+G(d,p)]

n	O–C bond order
0	0.881
1	0.467
2	0.721

[1] I. Mayer, *J. Comput. Chem.* **2007**, 28, 204-221.

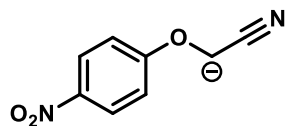
Figure S2: Highest occupied localized molecular orbital (HOLMO) of reactants **1a**, **1b** and **1c**
[ω B97X-D/6-31+G(d,p)]



Computational Details

All structures and energies reported were determined at the ω B97-XD/6-31+G(d,p) level with SMD water solvation using GAMESS [1 May 2012 (R1)]. Cartesian coordinates are given in Angstrom.

C1-1a



C1-1a

Energy: $-1687728.922 \text{ kJ mol}^{-1}$

Gibbs free energy: $-1687512.725 \text{ kJ mol}^{-1}$

C	6.0	-0.9998753315	0.0253725143	0.5814829142
C	6.0	-3.2124395929	-0.8498544487	0.2690286412
O	8.0	-2.2929634234	0.0576376670	0.9140360800
C	6.0	-3.8835872918	-0.2942474474	-0.8146571049
N	7.0	-4.4162881182	0.1145509870	-1.7879616208
C	6.0	-0.1356814696	0.8072173936	1.3735323264
C	6.0	1.2201382599	0.8268051705	1.1163519667
C	6.0	1.7251548093	0.0681668397	0.0554316490
C	6.0	0.8813018700	-0.6956434158	-0.7504517999
C	6.0	-0.4796410943	-0.7140249408	-0.4935311145
N	7.0	3.1467635913	0.0782758956	-0.2093163738
O	8.0	3.8756765432	0.7409560422	0.5272191289
O	8.0	3.5740583956	-0.5763233569	-1.1589747001
H	1.0	-3.8299197920	-1.3267240511	1.0248323854
H	1.0	-0.5497523435	1.3848295858	2.1937220386
H	1.0	1.8897284007	1.4180321306	1.7294882771
H	1.0	1.2887735250	-1.2708543871	-1.5737224083
H	1.0	-1.1538493762	-1.2959947795	-1.1082988593

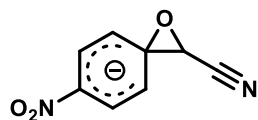
TS1-1a (conformer A)Energy: $-1687673.661 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1687458.89 \text{ kJ mol}^{-1}$ Imaginary frequency: $513.42i \text{ cm}^{-1}$

C	6.0	-1.1114832469	-0.6011967954	0.4780568006
C	6.0	-2.7906855367	-0.6420927763	-0.4302132061
O	8.0	-2.3636908270	-0.9601452425	0.9002600039
C	6.0	-3.4894065053	0.5511143811	-0.5908372465
N	7.0	-4.0100398146	1.5949537558	-0.7449530667
C	6.0	-0.5979897799	0.6912676761	0.8014557752
C	6.0	0.7150900168	0.9987188359	0.5455402284
C	6.0	1.5803651819	0.0217198529	0.0151586658
C	6.0	1.1169954375	-1.2925007467	-0.1999329218
C	6.0	-0.1935119679	-1.6091126520	0.0512940801
N	7.0	2.9371419630	0.3413480982	-0.2394286408
O	8.0	3.3386644196	1.4923175366	-0.0115183440
O	8.0	3.6894908683	-0.5371584391	-0.6867489668
H	1.0	-3.0047416002	-1.4923867590	-1.0672885529
H	1.0	-1.2677355325	1.4321692978	1.2252877581
H	1.0	1.0986439331	1.9871906885	0.7710213609
H	1.0	1.8073777175	-2.0538910153	-0.5441833311
H	1.0	-0.5579242579	-2.6206832540	-0.0971480956

TS1-1a (conformer B)Energy: $-1687674.545 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1687458.699 \text{ kJ mol}^{-1}$ Imaginary frequency: $520.05i \text{ cm}^{-1}$

C	6.0	1.1185209912	-0.6177658239	0.5116264677
C	6.0	2.7761907113	-0.6524276048	-0.4257990217
C	6.0	3.4247162034	0.5625454754	-0.6226312517
N	7.0	3.8895264586	1.6265172155	-0.8141518671
O	8.0	2.3794091088	-0.9715509468	0.9131421229
C	6.0	0.1956392716	-1.6231542023	0.0871930971
C	6.0	-1.1062812034	-1.2922690262	-0.1871243063
C	6.0	-1.5604176621	0.0279517627	0.0143188583
C	6.0	-0.6981196717	0.9955326994	0.5660029019
C	6.0	0.6068616344	0.6733115254	0.8454986601
N	7.0	-2.9043974979	0.3606461575	-0.2833776572
O	8.0	-3.6488617279	-0.5127847026	-0.7544523438
O	8.0	-3.3036186126	1.5161468452	-0.0722036988
H	1.0	2.9783256061	-1.4996425482	-1.0704310835
H	1.0	0.5526924800	-2.6383787341	-0.0542265470
H	1.0	-1.8009335210	-2.0464749903	-0.5384216563
H	1.0	-1.0764848791	1.9862554071	0.7912773230
H	1.0	1.2765531732	1.4037934980	1.2865802272

C2-1a (conformer A)



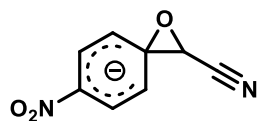
C2-1a

Energy: $-1687721.694 \text{ kJ mol}^{-1}$

Gibbs free energy: $-1687502.376 \text{ kJ mol}^{-1}$

C	6.0	-1.2029502161	-0.4744056466	0.0996206554
C	6.0	-2.6494919406	-0.6772618765	-0.1686006912
O	8.0	-2.1833428352	-0.9450012265	1.1409361102
C	6.0	-3.5413132198	0.4651320740	-0.3033348735
N	7.0	-4.2435502167	1.3798325214	-0.4167298878
C	6.0	-0.6382961347	0.8644025068	0.3351905198
C	6.0	0.7033462289	1.0668318973	0.3457213598
C	6.0	1.6159261976	0.0151590184	0.0313537489
C	6.0	1.0912233840	-1.2591881615	-0.3427739382
C	6.0	-0.2438751331	-1.4961721016	-0.3543683049
N	7.0	2.9755193599	0.2454635878	0.0159904588
O	8.0	3.4222867996	1.3758333619	0.3357685796
O	8.0	3.7616419758	-0.6779449654	-0.3141399672
H	1.0	-2.9752648923	-1.5363435269	-0.7559357793
H	1.0	-1.3177033192	1.6821898535	0.5577584232
H	1.0	1.0999527902	2.0522263949	0.5649300368
H	1.0	1.7832800166	-2.0384491822	-0.6437719991
H	1.0	-0.6306612307	-2.4660842497	-0.6536519126

C2-1a (conformer B)



C2-1a

Energy: $-1687721.875 \text{ kJ mol}^{-1}$

Gibbs free energy: $-1687502.177 \text{ kJ mol}^{-1}$

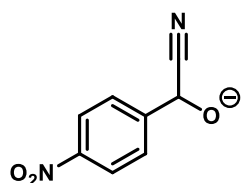
C	6.0	1.2049683064	0.4699673765	-0.1048493375
O	8.0	2.1982835067	0.9041800480	-1.1474711104
C	6.0	2.6487319083	0.6805866690	0.1757481177
C	6.0	3.5386484897	-0.4559152727	0.3602392343
N	7.0	4.2394937449	-1.3661057391	0.5121290099
C	6.0	0.2414101732	1.5072706329	0.3027441322
C	6.0	-1.0931658425	1.2673606964	0.2956263592
C	6.0	-1.6142546509	-0.0234781144	-0.0230804019
C	6.0	-0.6989788432	-1.0828191728	-0.3019028058
C	6.0	0.6419429137	-0.8760151853	-0.3024272041
N	7.0	-2.9733921757	-0.2550298457	-0.0005958036
O	8.0	-3.7616238219	0.6880712779	0.2624349851
O	8.0	-3.4177305084	-1.4051351147	-0.2453028731
H	1.0	2.9667488187	1.5592113337	0.7378694508
H	1.0	0.6254179669	2.4885598398	0.5663484593
H	1.0	-1.7877077349	2.0562774712	0.5639694605
H	1.0	-1.0932033233	-2.0752917101	-0.4917925532
H	1.0	1.3232323681	-1.6974373128	-0.5049595767

TS2-1a (conformer A)Energy: $-1687719.684 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1687501.346 \text{ kJ mol}^{-1}$ Imaginary frequency: $376.14i \text{ cm}^{-1}$

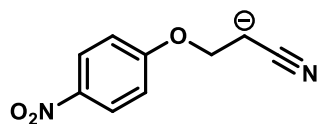
C	6.0	-1.1930730298	0.4252592171	0.0016771333
O	8.0	-2.2375286527	0.8854443163	-1.1986375529
C	6.0	-2.6366520151	0.6663075082	0.1242338175
C	6.0	-3.5382408971	-0.4691007727	0.3520914201
N	7.0	-4.2534471469	-1.3635170798	0.5286783586
C	6.0	-0.6367187770	-0.9016786258	-0.2067604504
C	6.0	0.7117996284	-1.0946124412	-0.2318730016
C	6.0	1.6094819703	-0.0220466586	0.0177544721
C	6.0	1.0848892424	1.2536888522	0.3586997578
C	6.0	-0.2595247013	1.4698709080	0.3914026734
N	7.0	2.9850357605	-0.2322397930	-0.0065202990
O	8.0	3.4336199104	-1.3657645691	-0.2887646824
O	8.0	3.7574429735	0.7179492266	0.2494609200
H	1.0	-2.9781607515	1.5412344280	0.6857842636
H	1.0	-1.3101358627	-1.7363319720	-0.3762844371
H	1.0	1.1137704174	-2.0840014635	-0.4210803136
H	1.0	1.7712430800	2.0518384419	0.6190078780
H	1.0	-0.6534086423	2.4409256148	0.6761098701

TS2-1a (conformer B)Energy: $-1687719.77 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1687502.224 \text{ kJ mol}^{-1}$ Imaginary frequency: $354.68i \text{ cm}^{-1}$

C	6.0	1.1890755560	0.4256336269	0.0222333175
O	8.0	2.1944404159	0.8930973145	-1.1987373579
C	6.0	2.6322201790	0.6837883291	0.1132150960
C	6.0	3.5587623320	-0.4366363999	0.3091825834
N	7.0	4.2933415173	-1.3207128164	0.4550488368
C	6.0	0.2501088667	1.4652574958	0.4170629601
C	6.0	-1.0928118178	1.2496922850	0.3506476573
C	6.0	-1.6095024454	-0.0288328812	0.0064232640
C	6.0	-0.7068265858	-1.1043064859	-0.2110128454
C	6.0	0.6408554439	-0.9092889433	-0.1616950828
N	7.0	-2.9846408251	-0.2416670832	-0.0303595603
O	8.0	-3.7604502419	0.7225797618	0.1501836425
O	8.0	-3.4291104358	-1.3905024995	-0.2474604294
H	1.0	2.9749045217	1.5624947088	0.6681847257
H	1.0	0.6384311671	2.4356401467	0.7115751446
H	1.0	-1.7855100050	2.0453071746	0.6023991200
H	1.0	-1.1051181046	-2.0968658106	-0.3911688291
H	1.0	1.3201991903	-1.7427692231	-0.3125603315

C3-1a**C3-1a**Energy: $-1687808.377 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1687588.323 \text{ kJ mol}^{-1}$

C	6.0	1.1026751942	0.3423866449	-0.2914350940
O	8.0	3.1332773247	0.0311437513	-1.6164938887
C	6.0	2.6187124576	0.5726338388	-0.5219238150
C	6.0	3.3082027115	0.0489413378	0.7413585764
N	7.0	3.9168567598	-0.3875869240	1.6303367688
C	6.0	0.4179241380	0.9455074126	0.7691714502
C	6.0	-0.9442027518	0.7444205538	0.9376352155
C	6.0	-1.6140937316	-0.0677315064	0.0228339327
C	6.0	-0.9593773479	-0.6719868536	-1.0462059465
C	6.0	0.4062850496	-0.4572367556	-1.1942378528
N	7.0	-3.0477269501	-0.2870051835	0.1922894522
O	8.0	-3.6031407796	0.2174689002	1.1628278870
O	8.0	-3.6360568289	-0.9682719078	-0.6410041026
H	1.0	2.7510152392	1.6804151583	-0.4267965258
H	1.0	0.9516470546	1.5802560731	1.4734339696
H	1.0	-1.4853483572	1.2066697507	1.7544243814
H	1.0	-1.5077298632	-1.2938997685	-1.7439874665
H	1.0	0.9646580451	-0.8975414444	-2.0138960073

C1-1b**C1-1b**Energy: $-1790969.091 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1790675.659 \text{ kJ mol}^{-1}$

C	6.0	-0.7379121246	-1.0160903930	-0.0846147306
C	6.0	-3.7353515821	0.2213171454	-0.4836163542
C	6.0	-3.1626566595	-0.8425535755	0.3507929720
O	8.0	-1.9503370204	-1.5473242776	-0.1999326105
C	6.0	-3.3216873059	1.5385429115	-0.4053442699
N	7.0	-2.9970008294	2.6736280772	-0.3134816067
C	6.0	-0.4505850110	0.2173682179	0.5321311369
C	6.0	0.8584351676	0.6612623801	0.6245298497
C	6.0	1.8916836551	-0.1128659604	0.1011512074
C	6.0	1.6287487945	-1.3359914992	-0.5241470326
C	6.0	0.3258314001	-1.7784833266	-0.6155313470
N	7.0	3.2556824414	0.3545875424	0.2036347325
O	8.0	3.4703321578	1.4305338977	0.7596874833
O	8.0	4.1512382687	-0.3426394581	-0.2706810486
H	1.0	-4.2936686745	-0.0645390552	-1.3709328106
H	1.0	1.0759540804	1.6105429816	1.0992328931
H	1.0	-1.2394082088	0.8430267490	0.9263731451
H	1.0	-3.8436399410	-1.6910213020	0.4353717889
H	1.0	-2.8929780049	-0.5186938082	1.3611063822
H	1.0	0.1005454603	-2.7261280494	-1.0935954919
H	1.0	2.4425462622	-1.9256277009	-0.9288470521

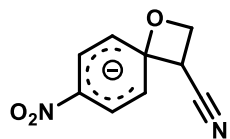
TS1-1b (conformer A)Energy: $-1790883.972 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1790593.134 \text{ kJ mol}^{-1}$ Imaginary frequency: $565.05i \text{ cm}^{-1}$

C	6.0	-0.9896895753	-0.8991295489	0.3387205754
C	6.0	-2.5790357498	-0.0718493111	-0.7388101056
C	6.0	-3.2087743429	-0.9174022484	0.3312489842
O	8.0	-2.0748784775	-1.6554802192	0.8273076101
C	6.0	-2.6311798120	1.3225716249	-0.6648292742
N	7.0	-2.5816816168	2.4910200051	-0.5552067335
C	6.0	-0.4368844325	0.1039575387	1.2006217741
C	6.0	0.8362885055	0.5737513362	1.0117970536
C	6.0	1.6602102471	-0.0014015319	0.0213675015
C	6.0	1.1987181983	-1.1091026636	-0.7196954674
C	6.0	-0.0786943118	-1.5729594764	-0.5350409751
N	7.0	2.9712918572	0.4866541995	-0.1783106790
O	8.0	3.3554191429	1.4711198782	0.4740997488
O	8.0	3.7084433513	-0.0748849750	-1.0054417573
H	1.0	-2.5359466592	-0.4814417934	-1.7452782874
H	1.0	1.2264154328	1.3682194467	1.6378638890
H	1.0	-1.0681584654	0.5283177667	1.9751714274
H	1.0	-3.9560636095	-1.6349061836	-0.0228692922
H	1.0	-3.6521239528	-0.3203602999	1.1378678435
H	1.0	-0.4423392594	-2.4266148494	-1.0984166024
H	1.0	1.8647367120	-1.5956100288	-1.4232290748

TS1-1b (conformer B)Energy: $-1790883.989 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1790592.961 \text{ kJ mol}^{-1}$ Imaginary frequency: $565.15i \text{ cm}^{-1}$

C	6.0	-0.9890444936	0.9009909195	0.3370215447
C	6.0	-2.5779739551	0.0738246771	-0.7411020577
C	6.0	-3.2081079419	0.9212748014	0.3272278379
O	8.0	-2.0740042131	1.6589048097	0.8236922276
C	6.0	-2.6303821860	-1.3204175869	-0.6650009647
N	7.0	-2.5806313936	-2.4886327550	-0.5532767113
C	6.0	-0.0765483217	1.5728982274	-0.5366663158
C	6.0	1.2005069826	1.1073940241	-0.7197317590
C	6.0	1.6600446238	-0.0001194908	0.0228805222
C	6.0	0.8346324882	-0.5731951237	1.0133061805
C	6.0	-0.4381315428	-0.1016895826	1.2005979891
N	7.0	2.9705677181	-0.4901666362	-0.1753958598
O	8.0	3.7095001568	0.0700893451	-1.0017979715
O	8.0	3.3524306956	-1.4750812824	0.4774675881
H	1.0	1.8676483851	1.5922570940	-1.4233217843
H	1.0	-0.4388381415	2.4262282848	-1.1014091822
H	1.0	-2.5334949750	0.4819499949	-1.7480988143
H	1.0	-3.6530462673	0.3256057259	1.1340819429
H	1.0	-3.9543098297	1.6391299316	-0.0286336999
H	1.0	-1.0705906331	-0.5243572664	1.9751765592
H	1.0	1.2232984320	-1.3674235642	1.6405998114

C2-1b (conformer A)

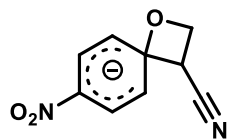


C2-1b

Energy: $-1790936.984 \text{ kJ mol}^{-1}$

Gibbs free energy: $-1790641.334 \text{ kJ mol}^{-1}$

C	6.0	-1.1124338913	-0.5647275160	0.0433994908
C	6.0	-2.5325152999	-0.1987696858	-0.5506667851
C	6.0	-3.1062057250	-1.0738248158	0.5718929039
O	8.0	-1.8077031310	-1.5837979226	0.8928510060
C	6.0	-2.9073360242	1.2030618263	-0.5880233116
N	7.0	-3.1999276303	2.3248196951	-0.6014630727
C	6.0	-0.4709025147	0.4773686525	0.8888484479
C	6.0	0.8650264861	0.7000924257	0.8946355985
C	6.0	1.7420316378	-0.0212515151	0.0278545912
C	6.0	1.1717703863	-0.9626141059	-0.8818070463
C	6.0	-0.1633667926	-1.1972414975	-0.9068361982
N	7.0	3.0967634092	0.2170042899	0.0418596691
O	8.0	3.5674364819	1.1052494031	0.8000449546
O	8.0	3.8622841735	-0.4544716155	-0.6987287799
H	1.0	-2.6703248956	-0.6287919363	-1.5456730325
H	1.0	1.2891241608	1.4391234542	1.5660746357
H	1.0	-1.1114021074	1.0372653193	1.5668525222
H	1.0	-3.7984995692	-1.8570926745	0.2517038016
H	1.0	-3.5470926381	-0.5090723640	1.4020690296
H	1.0	-0.5754042859	-1.9126707477	-1.6149110381
H	1.0	1.8275960816	-1.4793165339	-1.5747133753

C2-1b (conformer B)**C2-1b**Energy: $-1790937.001 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1790641.16 \text{ kJ mol}^{-1}$

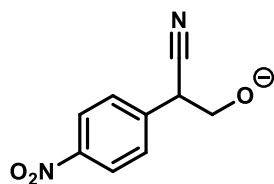
C	6.0	-1.1116683130	0.5667625441	0.0426733986
C	6.0	-2.5308117693	0.2003526843	-0.5531677137
C	6.0	-3.1060306640	1.0765413570	0.5675495109
O	8.0	-1.8080959684	1.5871407454	0.8894055907
C	6.0	-2.9059201123	-1.2014473318	-0.5895274523
N	7.0	-3.1988787659	-2.3231150872	-0.6015950327
C	6.0	-0.1610104891	1.1979994034	-0.9067793731
C	6.0	1.1736695699	0.9609551556	-0.8813641026
C	6.0	1.7419510290	0.0184208708	0.0282656297
C	6.0	0.8636497562	-0.6995642220	0.8964706418
C	6.0	-0.4718038266	-0.4742588150	0.8906455673
N	7.0	3.0957222644	-0.2243980428	0.0404060591
O	8.0	3.8627643994	0.4441392605	-0.7013941311
O	8.0	3.5643472828	-1.1142518453	0.7980783392
H	1.0	1.8308008738	1.4764313074	-1.5739630842
H	1.0	-0.5716315127	1.9141686211	-1.6148957341
H	1.0	-2.6670572242	0.6293214140	-1.5487636649
H	1.0	-3.5478860332	0.5128131823	1.3977915228
H	1.0	-3.7981241784	1.8590644194	0.2453400637
H	1.0	-1.1132432865	-1.0311966012	1.5701603043
H	1.0	1.2866506058	-1.4381171366	1.5691333605

TS2-1b (conformer A)Energy: $-1790908.898 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1790615.939 \text{ kJ mol}^{-1}$ Imaginary frequency: $413.99i \text{ cm}^{-1}$

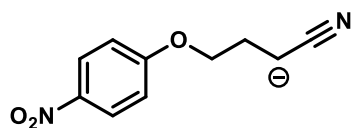
C	6.0	-1.0501119549	-0.3158329661	-0.1437181377
O	8.0	-1.8053907760	-1.7420345284	0.9003639304
C	6.0	-3.0003898629	-1.0543858444	0.7384066782
C	6.0	-2.5579727223	-0.1761434578	-0.4472037683
C	6.0	-3.0598843501	1.1945923660	-0.4984272362
N	7.0	-3.4775367350	2.2767947008	-0.4949874550
C	6.0	-0.4433578655	0.5877305030	0.7892888352
C	6.0	0.9193347507	0.7047178015	0.8844211227
C	6.0	1.7495828135	0.0029742163	-0.0125235023
C	6.0	1.1769977956	-0.7675791627	-1.0415924666
C	6.0	-0.1882648446	-0.8802136912	-1.1352647647
N	7.0	3.1587679361	0.1225950361	0.0808495141
O	8.0	3.6473933758	0.8477339563	0.9603896004
O	8.0	3.8713002223	-0.5051277064	-0.7170079146
H	1.0	-2.7900887298	-0.6555454571	-1.4030036468
H	1.0	1.3637893511	1.3485113491	1.6351206021
H	1.0	-1.0746623367	1.1451253966	1.4758427191
H	1.0	-3.8676003527	-1.6902665441	0.4990137472
H	1.0	-3.2816978538	-0.4290688800	1.6075564254
H	1.0	-0.6256717512	-1.4597483523	-1.9427438954
H	1.0	1.8204042977	-1.2449449106	-1.7720472423

TS2-1b (conformer B)Energy: $-1790909.99 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1790615.993 \text{ kJ mol}^{-1}$ Imaginary frequency: $410.21i \text{ cm}^{-1}$

C	6.0	-1.0481162774	-0.3508610149	0.1317125538
O	8.0	-1.8038722679	-1.7513465630	-0.9501087050
C	6.0	-2.9964835473	-1.0639177253	-0.7748961231
C	6.0	-2.5562204638	-0.2307103478	0.4422916650
C	6.0	-3.0641390262	1.1339100079	0.5575166929
N	7.0	-3.4847387642	2.2136444893	0.6085740481
C	6.0	-0.1785102969	-0.9190800357	1.1140518916
C	6.0	1.1853369391	-0.7764959180	1.0301103892
C	6.0	1.7473506771	0.0166600718	0.0137151848
C	6.0	0.9077604963	0.7089895302	-0.8833315576
C	6.0	-0.4525769782	0.5677511645	-0.7941528700
N	7.0	3.1535020652	0.1747625140	-0.0640285273
O	8.0	3.8735434247	-0.4076193935	0.7609819692
O	8.0	3.6324887914	0.8888870097	-0.9578150426
H	1.0	1.8339356641	-1.2526018148	1.7567998836
H	1.0	-0.6073963239	-1.5223649093	1.9085934262
H	1.0	-2.7830634867	-0.7557097554	1.3746491581
H	1.0	-3.2693296376	-0.4073912147	-1.6236789277
H	1.0	-3.8686757402	-1.7029799798	-0.5644991543
H	1.0	-1.0918247695	1.1206863941	-1.4769687486
H	1.0	1.3434393854	1.3693506678	-1.6247662518

C3-1b**C3-1b**Energy: $-1790980.934 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1790689.295 \text{ kJ mol}^{-1}$

C	6.0	-0.9266625148	0.0013360827	-0.3207408454
O	8.0	-2.5359171347	-2.3398604738	0.6784478959
C	6.0	-2.9898208208	-1.1035170218	0.7636187587
C	6.0	-2.4168193172	-0.1314412481	-0.4238612792
C	6.0	-3.1134623894	1.1438706391	-0.3773498212
N	7.0	-3.7162725703	2.1309839606	-0.2735365061
C	6.0	-0.3127829215	1.0866925966	0.3169267360
C	6.0	1.0668168433	1.1438779648	0.4604949517
C	6.0	1.8325528073	0.0902688178	-0.0299701280
C	6.0	1.2521779597	-1.0100322021	-0.6566574281
C	6.0	-0.1272179528	-1.0459039495	-0.7985370937
N	7.0	3.2831348704	0.1412006460	0.1133827012
O	8.0	3.7857515956	1.1516312608	0.5946066885
O	8.0	3.9390155468	-0.8286327459	-0.2528177932
H	1.0	-2.6925493792	-0.6333026992	-1.3568170276
H	1.0	1.5401053070	1.9896880654	0.9448312148
H	1.0	-0.9149107605	1.9036926681	0.7036417029
H	1.0	-4.0974700441	-0.9854554000	0.6531750360
H	1.0	-2.7177853948	-0.5461699136	1.6987018532
H	1.0	-0.5980175245	-1.8956899468	-1.2782300397
H	1.0	1.8724693670	-1.8157497270	-1.0297533769

C1-1c**C1-1c**Energy: $-1894144.208 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1893776.046 \text{ kJ mol}^{-1}$

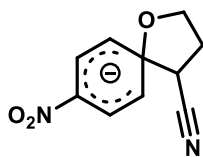
C	6.0	-0.3422944187	0.2682429977	-0.1904112844
C	6.0	-4.3153306937	-0.5962965994	1.1032490756
C	6.0	-3.9608803187	0.6165017663	0.2769503419
C	6.0	-2.5158583940	1.0935117919	0.3860994551
O	8.0	-1.6692590185	0.1119989409	-0.2268727624
C	6.0	-4.1676730078	-1.8753924212	0.6294730981
N	7.0	-4.0830046241	-2.9909146700	0.2182266653
C	6.0	0.4111560488	-0.7402123208	-0.8207272370
C	6.0	1.7889729486	-0.6741377285	-0.8401282037
C	6.0	2.4270476288	0.4052553601	-0.2212945286
C	6.0	1.6994058954	1.4113468577	0.4064214793
C	6.0	0.3131964524	1.3493875209	0.4208893203
N	7.0	3.8749786853	0.4789352499	-0.2370960854
O	8.0	4.4976932782	-0.3899397390	-0.8424650187
O	8.0	4.4210081716	1.4074150563	0.3539489065
H	1.0	-0.1087664231	-1.5686932230	-1.2901849120
H	1.0	-4.3889783404	-0.4749351161	2.1821608840
H	1.0	2.3704966218	-1.4474813745	-1.3267765957
H	1.0	-2.2357716867	1.2060865800	1.4410094144
H	1.0	-2.3739976902	2.0536099301	-0.1298028620
H	1.0	-4.5780551341	1.4736222680	0.5804826825
H	1.0	-4.1813978631	0.4502116573	-0.7856155535
H	1.0	-0.2418767987	2.1412740282	0.9072960782
H	1.0	2.2102193257	2.2428143859	0.8774590442

TS1-1c (conformer A – pseudo-equatorial)Energy: $-1894109.443 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1893745.264 \text{ kJ mol}^{-1}$ Imaginary frequency: $358.49i \text{ cm}^{-1}$

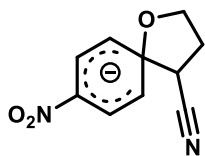
C	6.0	-0.8475091229	0.7863105402	-0.5340088429
C	6.0	-2.2412030636	-0.3950658802	0.9281010695
C	6.0	-3.4681564696	0.3197132922	0.4364698320
C	6.0	-3.0210185167	1.6459973407	-0.1867974817
O	8.0	-1.9572417559	1.3624132608	-1.0874609896
C	6.0	-1.9860175500	-1.7175272135	0.6000188689
N	7.0	-1.6801885375	-2.8076547742	0.2690794679
C	6.0	-0.1815426579	-0.1643968036	-1.3635552117
C	6.0	1.1012076159	-0.5570490847	-1.0885904827
C	6.0	1.8119188864	0.0392061552	-0.0256687632
C	6.0	1.2263889318	1.1028113933	0.7023140551
C	6.0	-0.0528642400	1.4993941583	0.4275899684
N	7.0	3.1234930244	-0.3795308192	0.2623743799
O	8.0	3.6489921960	-1.2621815439	-0.4412733635
O	8.0	3.7324511078	0.1368312814	1.2178641118
H	1.0	-0.7368924422	-0.6169227150	-2.1776971313
H	1.0	-1.8157729404	-0.0686642330	1.8741882815
H	1.0	1.5812966231	-1.3217002408	-1.6879497424
H	1.0	-2.6975860724	2.3541946507	0.5867735825
H	1.0	-3.8033695528	2.1221392734	-0.7817065227
H	1.0	-4.1929296266	0.5345767725	1.2329596065
H	1.0	-3.9843897156	-0.2723686603	-0.3266759956
H	1.0	-0.4924321948	2.3211316040	0.9828267164
H	1.0	1.8083575252	1.6127431066	1.4614934165

TS1-1c (conformer B – pseudo-axial)Energy: $-1894108.138 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1893741.655 \text{ kJ mol}^{-1}$ Imaginary frequency: $365.55i \text{ cm}^{-1}$

C	6.0	-2.2684963210	0.3158468262	1.0330497097
C	6.0	-0.8296275998	-0.9582954269	-0.2885506326
N	7.0	-1.5751007141	2.7162188280	0.4530596540
C	6.0	-1.9280268022	1.6336036632	0.7568846381
C	6.0	-3.5030424985	-0.2971154209	0.4221891659
C	6.0	-3.1098150477	-1.0064803208	-0.8828951518
O	8.0	-1.9084830444	-1.7235222976	-0.6361981967
C	6.0	-0.2873062379	-0.0069564140	-1.2127676016
C	6.0	0.9870811553	0.4664482023	-1.0582006464
C	6.0	1.8181765052	-0.0427962675	-0.0353721668
C	6.0	1.3516560050	-1.0937693110	0.7881667657
C	6.0	0.0756521785	-1.5640571762	0.6406592572
N	7.0	3.1228673631	0.4534254448	0.1273747806
O	8.0	3.8556131684	-0.0356557650	1.0082141285
O	8.0	3.5212967676	1.3761905814	-0.6081735449
H	1.0	-1.9308654251	-0.0564028696	1.9951727835
H	1.0	-4.2957526024	0.4292077459	0.2039139815
H	1.0	-3.9224865760	-1.0385112158	1.1097498850
H	1.0	-2.9723113959	-0.2832902586	-1.6964813034
H	1.0	-3.8463002967	-1.7460473728	-1.2052975434
H	1.0	-0.9079511152	0.3771156497	-2.0142889299
H	1.0	1.3760842322	1.2167740215	-1.7370798699
H	1.0	2.0161749810	-1.5248163660	1.5278948555
H	1.0	-0.2962756247	-2.3670091216	1.2689454616

C2-1c (conformer A – pseudo-equatorial)**C2-1c**Energy: $-1894197.114 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1893827.013 \text{ kJ mol}^{-1}$

C	6.0	-1.0301235606	0.5199103299	0.0664128962
C	6.0	-2.3377886713	-0.1944971207	0.5487196769
C	6.0	-3.3683877480	0.1472172237	-0.5412315676
C	6.0	-2.8550259400	1.5047345011	-1.0639811005
O	8.0	-1.6067918265	1.7626782678	-0.4235510407
C	6.0	-2.1751270607	-1.6241634059	0.7793874785
N	7.0	-2.0525489886	-2.7619993508	0.9634685797
C	6.0	-0.3349478755	-0.2209775419	-1.0421628576
C	6.0	1.0050636041	-0.3884248401	-1.0910663578
C	6.0	1.8532674632	0.0644044516	-0.0280221332
C	6.0	1.2400203244	0.6713189326	1.1162052896
C	6.0	-0.0973093591	0.8524562100	1.1885643534
N	7.0	3.2076697756	-0.1108432910	-0.0854547598
O	8.0	3.7295188202	-0.6910971186	-1.0801346896
O	8.0	3.9410499480	0.3097209962	0.8544094049
H	1.0	-0.9476726171	-0.5831241073	-1.8650860175
H	1.0	-2.6367407547	0.2568996100	1.5015963312
H	1.0	1.4634488329	-0.8858155204	-1.9395438895
H	1.0	-3.5265164719	2.3296745806	-0.8109168080
H	1.0	-2.7298695466	1.4866260863	-2.1535717720
H	1.0	-4.3798491823	0.2061167421	-0.1356870333
H	1.0	-3.3695656025	-0.6076178341	-1.3316254518
H	1.0	-0.5399974095	1.3063245016	2.0722698021
H	1.0	1.8743765930	0.9646333620	1.9461834405

C2-1c (conformer B – pseudo-axial)**C2-1c**Energy: $-1894192.757 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1893820.349 \text{ kJ mol}^{-1}$

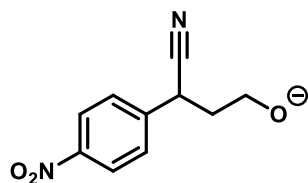
C	6.0	-2.0655578970	0.4062571117	0.8172269959
C	6.0	-0.9328272439	-0.2161604118	-0.0756172926
N	7.0	-3.1107667714	2.5580011208	-0.2599528614
C	6.0	-2.6449911559	1.6073734425	0.2124238269
C	6.0	-3.1004744073	-0.7297436940	0.8905107101
C	6.0	-2.9377747575	-1.4343013211	-0.4671904363
O	8.0	-1.7134900945	-0.9755909829	-1.0407076659
C	6.0	-0.1098433650	0.7782017766	-0.8363965784
C	6.0	1.2408862817	0.7951523044	-0.8186225481
C	6.0	1.9981280322	-0.1320959693	-0.0314354052
C	6.0	1.2795980442	-1.0957436856	0.7489543567
C	6.0	-0.0712834132	-1.1335944798	0.7526735862
N	7.0	3.3643325881	-0.0986530429	-0.0371804305
O	8.0	4.0250114706	-0.9308837635	0.6483877819
O	8.0	3.9688562929	0.7676942059	-0.7312740639
H	1.0	-1.6760303028	0.6910054885	1.7981872036
H	1.0	-4.1176925513	-0.3717649815	1.0595282478
H	1.0	-2.8439563250	-1.3914577122	1.7206029618
H	1.0	-3.7463045938	-1.1794805485	-1.1605666869
H	1.0	-2.9144589719	-2.5238682824	-0.3524323394
H	1.0	-0.6517950950	1.4865013570	-1.4571685497
H	1.0	1.7813492822	1.5246756110	-1.4123892342
H	1.0	1.8456773525	-1.8026043847	1.3468752843
H	1.0	-0.5796068300	-1.8849311281	1.3527229238

TS2-1c (conformer A – pseudo-equatorial)Energy: -1894130.917 kJ mol⁻¹Gibbs free energy: -1893764.042 kJ mol⁻¹Imaginary frequency: 223.08i cm⁻¹

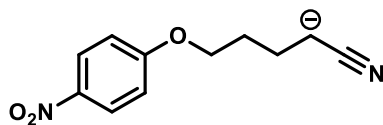
C	6.0	0.7936656341	-0.0462308842	0.3605785969
O	8.0	1.5838963432	-1.0132097537	-1.4143125516
C	6.0	2.8938450308	-1.2486997678	-1.1056416506
C	6.0	3.0665700976	-1.1716747229	0.4215264107
C	6.0	2.2267546089	0.0332949985	0.8891749903
C	6.0	2.8948502607	1.2824447698	0.5031204560
N	7.0	3.4466865768	2.2603753394	0.2170647467
C	6.0	0.1445418414	1.0752722543	-0.2175822520
C	6.0	-1.2183943171	1.0939467129	-0.4068369054
C	6.0	-1.9983768167	0.0155198959	0.0380514986
C	6.0	-1.3987689751	-1.0555249055	0.7202688735
C	6.0	-0.0362021976	-1.0658596986	0.9024757426
N	7.0	-3.4094753382	0.0286826885	-0.1639095953
O	8.0	-3.9218677721	0.9868328268	-0.7560254026
O	8.0	-4.0838968252	-0.9214387616	0.2527756413
H	1.0	0.7357783920	1.9158297747	-0.5658451279
H	1.0	2.1781173562	0.0488235996	1.9855224942
H	1.0	-1.6951678381	1.9402582109	-0.8881005062
H	1.0	3.2577429697	-2.2463529905	-1.4336437879
H	1.0	3.5956567430	-0.5132894312	-1.5663339106
H	1.0	2.6546920966	-2.0690213543	0.8943212390
H	1.0	4.1093520322	-1.0726668194	0.7435975866
H	1.0	0.4163316995	-1.8879139624	1.4483669506
H	1.0	-2.0135718315	-1.8580568166	1.1106882433

TS2-1c (conformer B – pseudo-axial)Energy: $-1894133.868 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1893769.271 \text{ kJ mol}^{-1}$ Imaginary frequency: $227.99i \text{ cm}^{-1}$

C	6.0	0.8825644303	-0.0245386654	-0.2093416537
O	8.0	1.5125901115	-2.0732885012	0.0320605529
C	6.0	2.8665882636	-1.9973653022	0.2089972607
C	6.0	3.2511945874	-0.5455502221	0.5517680209
C	6.0	2.3668739407	0.3020421872	-0.3766304198
C	6.0	2.5914338002	1.7379927798	-0.1746252865
N	7.0	2.7746519074	2.8712073627	-0.0108694871
C	6.0	0.2401558777	0.2432823866	1.0287245813
C	6.0	-1.1310204740	0.2330624268	1.1377431942
C	6.0	-1.9148645534	0.0138502272	-0.0062111718
C	6.0	-1.3099752335	-0.1342103043	-1.2640913623
C	6.0	0.0622879777	-0.1104887264	-1.3636957240
N	7.0	-3.3378290068	-0.0042670595	0.1031194979
O	8.0	-3.8552710873	0.2010316315	1.2076976318
O	8.0	-4.0145262836	-0.2296549449	-0.9076752681
H	1.0	0.5289963465	-0.2121802113	-2.3389579864
H	1.0	2.6533656562	0.0882148164	-1.4137273363
H	1.0	3.0191171634	-0.3149342695	1.5976166431
H	1.0	4.3123490658	-0.3304014371	0.3849879480
H	1.0	3.2456090576	-2.6524917248	1.0225993626
H	1.0	3.4446701654	-2.2858777212	-0.7003622697
H	1.0	0.8379084185	0.4256107285	1.9165442929
H	1.0	-1.6099397423	0.4037267910	2.0948503126
H	1.0	-1.9269275705	-0.2461909055	-2.1484076592

C3-1c**C3-1c**Energy: $-1894153.859 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1893789.057 \text{ kJ mol}^{-1}$

C	6.0	0.6584068228	0.2834795588	-0.0262542065
O	8.0	2.4972703258	-2.4140923868	-1.2853997236
C	6.0	3.4032427719	-1.9584527111	-0.3894131621
C	6.0	2.8410336062	-0.9311989959	0.6260673266
C	6.0	2.1780798461	0.2731477772	-0.1166126518
C	6.0	2.7661804938	1.5420984560	0.3144122371
N	7.0	3.2489986589	2.5389236774	0.6570044832
C	6.0	-0.0752773096	1.3275650034	0.5387898276
C	6.0	-1.4638772753	1.2637443834	0.5922224163
C	6.0	-2.1012287793	0.1484058542	0.0625242528
C	6.0	-1.3909974426	-0.9065386667	-0.5089924543
C	6.0	-0.0070465049	-0.8367419123	-0.5429789089
N	7.0	-3.5601512737	0.0793293032	0.1117934805
O	8.0	-4.1643176990	0.9563689530	0.7197527104
O	8.0	-4.1165204336	-0.8542283705	-0.4562029473
H	1.0	0.6176024277	-1.6379706716	-0.9543114006
H	1.0	2.4268756245	0.1578237976	-1.1810561212
H	1.0	2.0822475327	-1.4095185565	1.2548543467
H	1.0	3.6389658391	-0.5747835920	1.2892177181
H	1.0	3.8614231136	-2.7589437838	0.2469558000
H	1.0	4.2863547168	-1.4504925877	-0.8657367811
H	1.0	0.4237665916	2.2021596826	0.9451351301
H	1.0	-2.0397272390	2.0655271704	1.0375546040
H	1.0	-1.9142166551	-1.7660581388	-0.9109274520

C1-1d**C1-1d**Energy: -1997337.925 kJ mol⁻¹Gibbs free energy: -1996902.506 kJ mol⁻¹

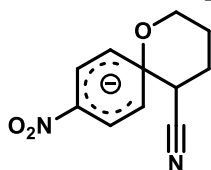
C	6.0	0.0653803762	-0.6612381823	-0.4225925378
C	6.0	4.3108704915	1.6159560160	0.8255019068
C	6.0	4.0964044678	0.7139383983	-0.3689548746
C	6.0	3.6905218694	-0.7271871226	-0.0079143901
C	6.0	2.2716353352	-0.8480731266	0.5034901418
O	8.0	1.3888212213	-0.6166343638	-0.6084038902
C	6.0	3.7223057227	2.8416524828	0.9664261667
N	7.0	3.2294116096	3.9182785452	1.1272564577
C	6.0	-0.5521481584	-0.9232392892	0.8100824699
C	6.0	-1.9370552337	-0.9553570397	0.8932647573
C	6.0	-2.6998828839	-0.7225020224	-0.2468407927
C	6.0	-2.0990905823	-0.4564011188	-1.4807162981
C	6.0	-0.7223552570	-0.4282496797	-1.5654988136
N	7.0	-4.1466413832	-0.7589779945	-0.1543045733
O	8.0	-4.6572247121	-1.0363096050	0.9280237142
O	8.0	-4.8037440754	-0.5111273444	-1.1624210410
H	1.0	5.1815086637	1.4329013549	1.4529325495
H	1.0	-2.4192793735	-1.1614337065	1.8410376172
H	1.0	0.0315229418	-1.1031178182	1.7040768275
H	1.0	2.0780676223	-1.8486027318	0.9080874270
H	1.0	2.0847593574	-0.0955500894	1.2790729956
H	1.0	3.8073609186	-1.3922227601	-0.8734498288
H	1.0	4.3580586027	-1.1025128522	0.7771217896
H	1.0	3.3289875082	1.1404339532	-1.0272084700
H	1.0	5.0075827844	0.6466368712	-0.9841931815
H	1.0	-0.2304814031	-0.2270418126	-2.5111465163
H	1.0	-2.7084261579	-0.2762594176	-2.3582109758

TS1-1d (conformer A – equatorial)Energy: -1997284.741 kJ mol⁻¹Gibbs free energy: -1996843.848 kJ mol⁻¹Imaginary frequency: 371.04i cm⁻¹

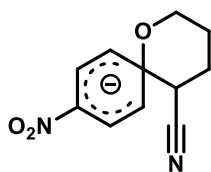
C	6.0	0.7459010860	-0.8790781848	-0.3547525155
C	6.0	1.9571852822	0.8901714893	0.6415291797
C	6.0	3.2540208054	0.7677980806	-0.1328640612
C	6.0	3.9304857620	-0.5867947602	0.1191596757
C	6.0	2.9170182394	-1.7276972477	0.1898380258
O	8.0	1.8730695793	-1.5294771107	-0.7679565411
C	6.0	1.1446776067	1.9863991666	0.3758401644
N	7.0	0.4188434486	2.8614056247	0.0632171744
C	6.0	-0.0099882291	-1.3516334837	0.7733796594
C	6.0	-1.3054911074	-0.9573289594	0.9535999719
C	6.0	-1.9491480318	-0.1543695354	-0.0182783053
C	6.0	-1.2677022592	0.1827469851	-1.2075188320
C	6.0	0.0270134342	-0.2220229753	-1.3965095919
N	7.0	-3.2729702366	0.2622057595	0.1824136609
O	8.0	-3.8601355019	-0.0616343776	1.2340773944
O	8.0	-3.8387847028	0.9525192357	-0.6880004914
H	1.0	1.9623807959	0.5708838499	1.6830772806
H	1.0	-1.8603812801	-1.2807980600	1.8265708688
H	1.0	0.4620201442	-1.9853923973	1.5162003484
H	1.0	3.3758890725	-2.6889547209	-0.0532700180
H	1.0	2.4963147450	-1.8107304501	1.1951835389
H	1.0	4.6630320039	-0.7798372846	-0.6720182151
H	1.0	4.4819275780	-0.5678586604	1.0674997392
H	1.0	3.0248685866	0.8538998702	-1.2033770752
H	1.0	3.9750676824	1.5686581057	0.0889059567
H	1.0	0.5571177879	0.0196390117	-2.3118865145
H	1.0	-1.7852985654	0.7406815251	-1.9788931173

TS1-1d (conformer B – axial)Energy: -1997287.445 kJ mol⁻¹Gibbs free energy: -1996848.069 kJ mol⁻¹Imaginary frequency: 409.77i cm⁻¹

C	6.0	0.5738325788	-0.8122083481	0.5015588111
C	6.0	1.7348553979	0.4317959754	-1.1102598102
C	6.0	2.9200942739	-0.4931353649	-1.2810238572
C	6.0	3.7411398886	-0.6393262830	0.0098078606
C	6.0	2.8451725449	-0.7066854462	1.2461589724
O	8.0	1.6723140015	-1.4773053510	0.9659493953
C	6.0	1.9122693255	1.7021703411	-0.5716951467
N	7.0	2.0055442032	2.7366861316	-0.0119446873
C	6.0	-0.0469082542	0.2203633671	1.2776487732
C	6.0	-1.3201929477	0.6265733632	0.9872255726
C	6.0	-2.0728663124	-0.0420559788	-0.0059406798
C	6.0	-1.5447735213	-1.1917994564	-0.6327173766
C	6.0	-0.2683272605	-1.5955628026	-0.3496183453
N	7.0	-3.3795632738	0.3893950369	-0.3060656422
O	8.0	-3.8328656966	1.3977938941	0.2653077651
O	8.0	-4.0526768309	-0.2407757001	-1.1419151276
H	1.0	-1.7720316978	1.4462346829	1.5336392602
H	1.0	0.5166493646	0.7291262630	2.0516947803
H	1.0	0.9448002446	0.3708594288	-1.8541841462
H	1.0	3.3465689177	-1.2087506513	2.0772591678
H	1.0	2.5659383668	0.2958519996	1.5816005006
H	1.0	4.3623335453	-1.5394289040	-0.0551477758
H	1.0	4.4242723189	0.2098276507	0.1325243586
H	1.0	2.5199852018	-1.4769498675	-1.5545778543
H	1.0	3.5926857474	-0.2028420369	-2.1016410829
H	1.0	0.1558091376	-2.4768443299	-0.8198026527
H	1.0	-2.1607721928	-1.7526045278	-1.3261047161

C2-1d (conformer A – equatorial)**C2-1d**Energy: $-1997386.637 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1996938.596 \text{ kJ mol}^{-1}$

C	6.0	0.8687738680	-0.3129433805	-0.0151204492
C	6.0	1.9897375694	0.6969180561	0.4515544063
C	6.0	3.2513243956	0.5752111364	-0.4223850790
C	6.0	3.8631530772	-0.8177152667	-0.2053539811
C	6.0	2.7545903061	-1.8329798764	0.1058402759
O	8.0	1.5497150643	-1.4792823030	-0.5588095814
C	6.0	1.4765776635	2.0653434151	0.4845283448
N	7.0	1.1035235458	3.1622364719	0.5213005597
C	6.0	-0.0007169232	-0.7048848742	1.1486875836
C	6.0	-1.3504259380	-0.6776773193	1.1103384904
C	6.0	-2.0594301068	-0.2017041358	-0.0411113571
C	6.0	-1.2932275855	0.2659743540	-1.1602502586
C	6.0	0.0561912723	0.2396275798	-1.1517451103
N	7.0	-3.4247974399	-0.1828700256	-0.0601158937
O	8.0	-4.0746935867	-0.6513007768	0.9190194922
O	8.0	-4.0427912058	0.2985550992	-1.0534550825
H	1.0	2.2620220025	0.4659045212	1.4906658540
H	1.0	-1.9260404195	-1.0010672046	1.9712086681
H	1.0	0.5017075240	-1.0539394353	2.0485447146
H	1.0	3.0163030988	-2.8329998712	-0.2472973349
H	1.0	2.5853009380	-1.9145894972	1.1895086239
H	1.0	4.4149897234	-1.1168161176	-1.1012468810
H	1.0	4.5782615167	-0.7944595818	0.6247545003
H	1.0	2.9724552148	0.7138863759	-1.4711371931
H	1.0	3.9688378918	1.3610783854	-0.1722093805
H	1.0	0.6100268246	0.5973616675	-2.0164641719
H	1.0	-1.8228961840	0.6498407412	-2.0260641227

C2-1d (conformer B – axial)**C2-1d**Energy: $-1997382.209 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1996934.44 \text{ kJ mol}^{-1}$

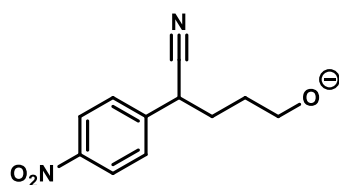
C	6.0	0.7148445008	-0.3076554824	0.0051512994
C	6.0	1.7981825080	0.3481181807	-0.9468414683
C	6.0	2.9917687398	-0.6026495568	-1.1490116953
C	6.0	3.6944481485	-0.8857571569	0.1867890370
C	6.0	2.6769829913	-0.8268406648	1.3353709482
O	8.0	1.3904571312	-1.2403674412	0.8971829919
C	6.0	2.2723429508	1.6551716720	-0.4739753931
N	7.0	2.6714028720	2.6825873404	-0.1143004352
C	6.0	-0.0468009378	0.7100423541	0.8106395514
C	6.0	-1.3958357526	0.7788810004	0.8410428608
C	6.0	-2.2134526335	-0.0891832254	0.0450624250
C	6.0	-1.5555179091	-1.0545925577	-0.7876505421
C	6.0	-0.2099290689	-1.1509858178	-0.8299829046
N	7.0	-3.5751791953	-0.0050962941	0.0885455012
O	8.0	-4.1326009715	0.8637535359	0.8199135407
O	8.0	-4.2834666015	-0.7947551178	-0.6010660183
H	1.0	-1.8863784644	1.5059772280	1.4795670410
H	1.0	0.5323245848	1.3779296535	1.4433356897
H	1.0	1.3050246474	0.5448012651	-1.9042145127
H	1.0	2.9535897563	-1.5035065882	2.1473295030
H	1.0	2.6273749188	0.1833733174	1.7670845776
H	1.0	4.1670539127	-1.8714732002	0.1435662290
H	1.0	4.4904967952	-0.1554118734	0.3700827147
H	1.0	2.5934952555	-1.5292630694	-1.5714231666
H	1.0	3.6847540951	-0.1909696832	-1.8876158172
H	1.0	0.2587582002	-1.8897092050	-1.4757398900
H	1.0	-2.1647438404	-1.7060685619	-1.4054147902

TS2-1d (conformer A – equatorial)Energy: $-1997311.264 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1996873.215 \text{ kJ mol}^{-1}$ Imaginary frequency: $223.20i \text{ cm}^{-1}$

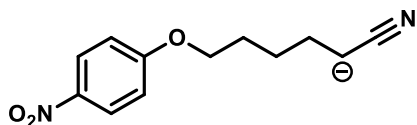
C	6.0	-0.6851364467	0.2018551973	-0.1530873099
O	8.0	-1.3210613857	-1.8685766319	0.4111302858
C	6.0	-2.4944834869	-2.1138717264	-0.2375475658
C	6.0	-3.6502124754	-1.2567262220	0.3224521285
C	6.0	-3.1570076719	0.1484867116	0.6900457146
C	6.0	-2.1287988451	0.6853109087	-0.3353661148
C	6.0	-2.1167569485	2.1557397449	-0.3181428017
N	7.0	-2.1161057054	3.3150577669	-0.2920728772
C	6.0	0.0747492363	-0.1038346668	-1.3043294763
C	6.0	1.4393177539	-0.2860897232	-1.2260860849
C	6.0	2.0876733411	-0.0941264846	0.0003946854
C	6.0	1.3702456325	0.3220675409	1.1334043669
C	6.0	0.0096169296	0.5027220757	1.0418969997
N	7.0	3.5051538774	-0.2760385240	0.0882198169
O	8.0	4.1264577489	-0.6295840891	-0.9196527859
O	8.0	4.0653210271	-0.0787890962	1.1716821059
H	1.0	-2.4631195530	0.4079384977	-1.3427997875
H	1.0	2.0120599101	-0.5607286076	-2.1040673768
H	1.0	-0.4287794050	-0.2425671175	-2.2565152213
H	1.0	-2.8080849419	-3.1809038737	-0.1906122928
H	1.0	-2.4204663297	-1.9059799629	-1.3378907809
H	1.0	-4.0556909254	-1.7210379196	1.2297957501
H	1.0	-4.4716094577	-1.1923568334	-0.4057039749
H	1.0	-2.6833548521	0.1354480786	1.6742871982
H	1.0	-4.0024730178	0.8415515609	0.7479217356
H	1.0	-0.5382319131	0.8422947681	1.9152892202
H	1.0	1.8928029519	0.5179163230	2.0620562422

TS2-1d (conformer B – axial)Energy: -1997307.261 kJ mol⁻¹Gibbs free energy: -1996869.191 kJ mol⁻¹Imaginary frequency: 271.48i cm⁻¹

C	6.0	0.5925522882	-0.0876103844	0.4406547567
O	8.0	1.1763357026	1.4404681222	-1.0222700103
C	6.0	2.3787383986	1.0297309573	-1.5258390376
C	6.0	3.5109125432	1.1580124065	-0.4825277114
C	6.0	2.9829121371	0.8451391524	0.9191468603
C	6.0	2.0057493681	-0.3536117784	0.9822757038
C	6.0	2.6263291705	-1.5502703172	0.3987913495
N	7.0	3.1451715775	-2.4950306582	-0.0271539517
C	6.0	-0.0383812514	-0.9995246039	-0.4399148140
C	6.0	-1.3972924571	-0.9463469035	-0.6620706917
C	6.0	-2.1820863652	-0.0297277874	0.0505707471
C	6.0	-1.5978877757	0.8009440883	1.0231389403
C	6.0	-0.2428433602	0.7398366659	1.2372589690
N	7.0	-3.5911761178	0.0187120692	-0.1708566168
O	8.0	-4.0937595934	-0.7470290499	-1.0021113341
O	8.0	-4.2707102764	0.8289731444	0.4711327821
H	1.0	-1.8637045452	-1.6185978997	-1.3731550791
H	1.0	0.5572569641	-1.7189988833	-0.9926152933
H	1.0	1.8744330515	-0.6075338155	2.0428690918
H	1.0	2.6808077390	1.5930046377	-2.4354651071
H	1.0	2.3479295986	-0.0369032266	-1.8631781145
H	1.0	3.9041936459	2.1822201713	-0.4721214790
H	1.0	4.3500911764	0.4951752455	-0.7366237270
H	1.0	2.4295913665	1.7036586549	1.3056657448
H	1.0	3.8101087269	0.6531292765	1.6107650732
H	1.0	0.2007835216	1.3636351257	2.0078130017
H	1.0	-2.2210340195	1.4607835692	1.6155658140

C3-1d**C3-1d**Energy: $-1997345.987 \text{ kJ mol}^{-1}$ Gibbs free energy: $-1996906.442 \text{ kJ mol}^{-1}$

C	6.0	0.4724275838	-0.4633507855	0.5324016927
O	8.0	1.8253128999	2.8838624253	-0.7212579795
C	6.0	2.5585932799	1.8798582297	-1.2656521129
C	6.0	3.5223365299	1.1939949112	-0.2730214397
C	6.0	2.8614831373	0.6083082654	0.9780419195
C	6.0	1.9692037309	-0.6536864338	0.8086849032
C	6.0	2.5294227160	-1.5681716028	-0.1991040371
N	7.0	2.9764028055	-2.2994992866	-0.9794479303
C	6.0	-0.3682475310	-1.5664294935	0.7377008099
C	6.0	-1.7340861282	-1.4742290993	0.5180129233
C	6.0	-2.2510870553	-0.2530177757	0.0959430865
C	6.0	-1.4409083341	0.8573321824	-0.1057939062
C	6.0	-0.0686071710	0.7539201178	0.1112908269
N	7.0	-3.6901638068	-0.1412403825	-0.1412156450
O	8.0	-4.3771680377	-1.1502557431	-0.0237274586
O	8.0	-4.1461956860	0.9541920991	-0.4482387575
H	1.0	-2.3878056248	-2.3232227324	0.6761725388
H	1.0	0.0444629145	-2.5137522472	1.0759684762
H	1.0	2.0299681000	-1.2106398036	1.7535323024
H	1.0	3.1963891004	2.2021896445	-2.1273547075
H	1.0	1.9288035905	1.0553357061	-1.7069325809
H	1.0	4.2391807027	1.9501419266	0.0744240826
H	1.0	4.1088057198	0.4167211367	-0.7858355718
H	1.0	2.2489167805	1.3788668188	1.4563836545
H	1.0	3.6441348114	0.3364440375	1.6935211550
H	1.0	0.5656949980	1.6409687883	-0.0732913346
H	1.0	-1.8736238851	1.7935026737	-0.4385186990

C1-1e**C1-1e**Energy: $-2100533.549 \text{ kJ mol}^{-1}$ Gibbs free energy: $-2100027.276 \text{ kJ mol}^{-1}$

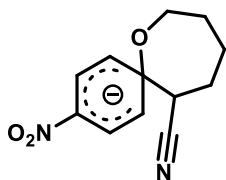
C	6.0	-0.5268535082	0.3019359149	0.8522688650
C	6.0	3.9825770557	-1.2351950625	-2.0846237783
C	6.0	4.0945507008	0.2482433250	-1.7875112687
C	6.0	4.2300422614	0.6275220328	-0.3027745042
C	6.0	3.1137560116	0.1178388551	0.6131012542
C	6.0	1.7392137540	0.5046592173	0.1065624506
O	8.0	0.7786729112	0.1497733898	1.1125640017
C	6.0	4.8404465181	-2.1555105038	-1.5457943848
N	7.0	5.5773961485	-2.9620317668	-1.0628685138
C	6.0	-1.0406778410	0.7924805926	-0.3581135509
C	6.0	-2.4142828295	0.8915892336	-0.5315541930
C	6.0	-3.2669783549	0.5110239385	0.4993081859
C	6.0	-2.7696529212	0.0344680910	1.7156521097
C	6.0	-1.4044406922	-0.0689299056	1.8873306810
N	7.0	-4.7018549330	0.6099523522	0.3081179979
O	8.0	-5.1237466760	1.0042657455	-0.7761531774
O	8.0	-5.4367399924	0.2930587813	1.2398582322
H	1.0	3.4135640772	-1.5507392812	-2.9553630543
H	1.0	-2.8185383625	1.2626337293	-1.4655043565
H	1.0	-0.3861628096	1.0963995509	-1.1647912227
H	1.0	1.6741612286	1.5850192882	-0.0822426999
H	1.0	1.5094141245	-0.0391383018	-0.8164397849
H	1.0	3.1679820774	-0.9720974111	0.6921217725
H	1.0	3.2514916846	0.5314915810	1.6189255759
H	1.0	5.1838070036	0.2460129196	0.0811688242
H	1.0	4.2868665464	1.7222519107	-0.2289586408
H	1.0	4.9465582146	0.7228781470	-2.3058953931
H	1.0	3.2058151865	0.7439869979	-2.2006042099
H	1.0	-0.9918866567	-0.4387869919	2.8199759112
H	1.0	-3.4491626417	-0.2518178391	2.5089011079

TS1-1e (conformer A – pseudo-equatorial)Energy: -2100479.611 kJ mol⁻¹Gibbs free energy: -2099965.96 kJ mol⁻¹Imaginary frequency: 387.74i cm⁻¹

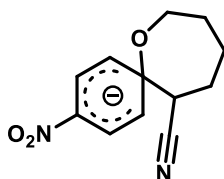
C	6.0	-0.4770058269	0.8584133209	0.1997241638
C	6.0	-1.5618520595	-0.8419642348	-0.8952618012
C	6.0	-3.0835841426	-0.9734867156	-0.8017268000
C	6.0	-3.8178957947	0.3738018077	-0.8744896394
C	6.0	-3.9206720785	1.1127590375	0.4659003316
C	6.0	-2.6148973822	1.1222512527	1.2406468914
O	8.0	-1.5760774021	1.6367291123	0.4079445130
C	6.0	-0.8207136728	-1.9668840377	-0.5096991628
N	7.0	-0.1620614584	-2.8456960234	-0.0897026351
C	6.0	0.1936128202	0.2183541793	1.2999248610
C	6.0	1.4916085139	-0.1951294559	1.1813796557
C	6.0	2.2406406910	0.1103840898	0.0206591803
C	6.0	1.6554511092	0.9137103223	-0.9906531848
C	6.0	0.3580990029	1.3183789694	-0.8805728854
N	7.0	3.5627516366	-0.3231550359	-0.1035070203
O	8.0	4.0828944177	-0.9920480570	0.8140514923
O	8.0	4.2041409229	-0.0389869149	-1.1373397891
H	1.0	1.9682850105	-0.7302474747	1.9946724180
H	1.0	-0.3529480668	0.0000998262	2.2107812749
H	1.0	-1.2284635219	-0.4366492271	-1.8510780909
H	1.0	-2.6822625579	1.7528124885	2.1339945019
H	1.0	-2.3681869100	0.1069970373	1.5624526308
H	1.0	-4.2628471490	2.1407471002	0.2973181531
H	1.0	-4.6714987293	0.6302927174	1.1055720247
H	1.0	-3.3089023795	1.0141666682	-1.6046906530
H	1.0	-4.8331415962	0.2162806594	-1.2566245082
H	1.0	-3.4496023559	-1.6057621961	-1.6246497409
H	1.0	-3.3646535471	-1.4983988556	0.1214415269
H	1.0	-0.0977936626	1.9396078521	-1.6451831549
H	1.0	2.2560431368	1.2201389392	-1.8391749438

TS1-1e (conformer B – pseudo-axial)Energy: -2100478.965 kJ mol⁻¹Gibbs free energy: -2099968.951 kJ mol⁻¹Imaginary frequency: 392.28i cm⁻¹

C	6.0	0.3555607919	0.4657385701	0.8390108602
C	6.0	1.3411461337	-0.7488203749	-0.9394492242
C	6.0	2.1543204707	0.2668603055	-1.7078780238
C	6.0	3.5419088593	0.5771952067	-1.1335758890
C	6.0	3.6175545889	0.7746930983	0.3892560000
C	6.0	2.5025688140	1.5985622814	1.0340437826
O	8.0	1.4590515536	0.7696647106	1.5615251919
C	6.0	1.9404957233	-1.8506372284	-0.3410191468
N	7.0	2.4028065865	-2.7615988489	0.2523907275
C	6.0	-0.3194301599	1.4404867748	0.0335481733
C	6.0	-1.5871828946	1.1925947682	-0.4248032557
C	6.0	-2.2775908335	0.0328671997	-0.0188038383
C	6.0	-1.7053916377	-0.8207568287	0.9540057813
C	6.0	-0.4385789543	-0.5829337257	1.4063192784
N	7.0	-3.5708884965	-0.2275034776	-0.5153473798
O	8.0	-4.0687258477	0.5503484009	-1.3486118026
O	8.0	-4.1833883316	-1.2342216272	-0.1173370474
H	1.0	0.3541268417	-0.9646780320	-1.3457335992
H	1.0	-2.0788518970	1.9010401159	-1.0820011185
H	1.0	0.1786638732	2.3549085383	-0.2641190450
H	1.0	2.8844460207	2.1276152387	1.9102737380
H	1.0	2.1060910045	2.3530309393	0.3474092038
H	1.0	3.6327905499	-0.1937473509	0.8995021822
H	1.0	4.5730587959	1.2594626076	0.6226075785
H	1.0	4.2378442288	-0.2276159689	-1.4003911865
H	1.0	3.9179941681	1.4786318372	-1.6336637556
H	1.0	2.2858260673	-0.0176856327	-2.7636484852
H	1.0	1.5633546260	1.1943733328	-1.7422322557
H	1.0	0.0196201767	-1.2260035770	2.1495601665
H	1.0	-2.2814463588	-1.6550811254	1.3370697437

C2-1e (conformer A – pseudo-equatorial)**C2-1e**Energy: $-2100583.934 \text{ kJ mol}^{-1}$ Gibbs free energy: $-2100064.063 \text{ kJ mol}^{-1}$

C	6.0	-0.7050253237	0.0414448366	-0.4479084332
O	8.0	-1.2680113931	1.1827766718	-1.1490356279
C	6.0	-1.6925271811	2.3221026211	-0.4186287878
C	6.0	-2.8661816303	2.0839775507	0.5440607154
C	6.0	-3.7232650501	0.8668867118	0.1890875242
C	6.0	-3.0960019922	-0.4712553101	0.5944107280
C	6.0	-1.9157051095	-0.9436421751	-0.2836109638
C	6.0	-1.4455433004	-2.2357178770	0.2313719525
N	7.0	-1.1085792466	-3.2514814313	0.6777253019
C	6.0	-0.0519589874	0.3834173057	0.8632471773
C	6.0	1.2881212810	0.3837502565	1.0431624606
C	6.0	2.1891350918	-0.0139016741	0.0044201010
C	6.0	1.6269494121	-0.5127260412	-1.2184960212
C	6.0	0.2931770496	-0.5422415450	-1.4136683249
N	7.0	3.5420317668	0.0090432472	0.1955408824
O	8.0	4.0240094143	0.3974349552	1.2985302749
O	8.0	4.3145593227	-0.3549670262	-0.7369634092
H	1.0	1.7026533378	0.6648574139	2.0059005464
H	1.0	-0.6908971082	0.6533269376	1.6982706658
H	1.0	-2.2929254763	-1.1280877721	-1.2983426762
H	1.0	-1.9947144996	3.0234541011	-1.2021819344
H	1.0	-0.8444170767	2.7716316025	0.1152417397
H	1.0	-3.4888969493	2.9859934990	0.5435114061
H	1.0	-2.5043050046	1.9687143801	1.5730675979
H	1.0	-3.9615980940	0.8650340352	-0.8816543269
H	1.0	-4.6771633067	0.9491097046	0.7215538341
H	1.0	-3.8638609360	-1.2512222439	0.5484678810
H	1.0	-2.7764490632	-0.4179272014	1.6421963319
H	1.0	-0.1112877739	-0.9455256666	-2.3397682640
H	1.0	2.2996888865	-0.8958746724	-1.9785348570

C2-1e (conformer B – pseudo-axial)**C2-1e**Energy: -2100582.385 kJ mol⁻¹Gibbs free energy: -2100057.731 kJ mol⁻¹

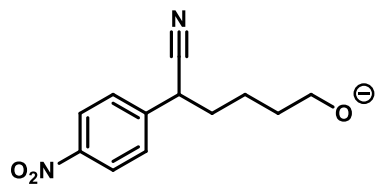
C	6.0	-0.5614268562	-0.1162714935	-0.1510022475
O	8.0	-1.3425952782	0.2675197185	-1.3096942369
C	6.0	-1.8069292918	1.6026440449	-1.4436629897
C	6.0	-2.7642829910	2.1004049027	-0.3476024666
C	6.0	-3.5054425936	0.9948975624	0.4083129993
C	6.0	-2.6415388683	0.2630600404	1.4415825263
C	6.0	-1.5887685908	-0.7163807685	0.8774815386
C	6.0	-2.2824728335	-1.8633444342	0.2734413055
N	7.0	-2.8477199125	-2.7674356104	-0.1816945630
C	6.0	0.2165906245	1.0121669877	0.4761429346
C	6.0	1.5653250727	1.0318739237	0.5714438323
C	6.0	2.3774463911	-0.0403580767	0.0829976283
C	6.0	1.7138098320	-1.1440086220	-0.5490799203
C	6.0	0.3694401774	-1.1949190678	-0.6482445520
N	7.0	3.7345761713	-0.0194153222	0.2274817770
O	8.0	4.2968504619	0.9603873240	0.7970486809
O	8.0	4.4328140221	-0.9822831460	-0.2035870332
H	1.0	-1.0125692854	-1.1212506509	1.7185206666
H	1.0	2.0574450578	1.8744707462	1.0464347294
H	1.0	-0.3380482581	1.8496748419	0.8845607157
H	1.0	-2.3283411057	1.5881158891	-2.4049679089
H	1.0	-0.9566531832	2.2911588814	-1.5431709270
H	1.0	-3.4925904467	2.7664266577	-0.8246275212
H	1.0	-2.2287577419	2.7204706697	0.3813882239
H	1.0	-3.9436524429	0.2779438211	-0.2971999032
H	1.0	-4.3430387545	1.4510299266	0.9473222910
H	1.0	-3.2872082869	-0.3069451937	2.1181048408
H	1.0	-2.1202092068	0.9949307255	2.0683967441
H	1.0	-0.1014832483	-2.0376098420	-1.1485657167
H	1.0	2.3178141303	-1.9504586794	-0.9511378275

TS2-1e (conformer A – pseudo-equatorial)Energy: -2100503.543 kJ mol⁻¹Gibbs free energy: -2099994.695 kJ mol⁻¹Imaginary frequency: 203.47i cm⁻¹

C	6.0	-0.5382632423	-0.4030345934	-0.1800064428
O	8.0	-1.2866776003	1.3032416394	-1.3399149639
C	6.0	-1.7808921801	2.4275572206	-0.7371474890
C	6.0	-2.6430423210	2.1588363995	0.5139403988
C	6.0	-3.6014859451	0.9776314505	0.3335179165
C	6.0	-3.0422320266	-0.4023891679	0.6965753890
C	6.0	-1.9548592921	-0.9794753547	-0.2375054714
C	6.0	-1.8484010027	-2.4274956746	0.0366265813
N	7.0	-1.7726168444	-3.5630391073	0.2597199946
C	6.0	0.0162614724	0.0720301221	1.0303351736
C	6.0	1.3692682686	0.3168507073	1.1465593220
C	6.0	2.2199754956	0.0220657707	0.0749424050
C	6.0	1.7140668575	-0.5698852598	-1.0945422644
C	6.0	0.3656261747	-0.8084496747	-1.1978092680
N	7.0	3.6230114585	0.2765590649	0.1921594691
O	8.0	4.0594625858	0.7495074050	1.2473167498
O	8.0	4.3568524083	0.0189495991	-0.7680236626
H	1.0	1.7793311789	0.7166897285	2.0666244748
H	1.0	-0.6233666238	0.2839416761	1.8785663420
H	1.0	-2.2955065321	-0.8760571390	-1.2718782070
H	1.0	-2.4273193813	3.0016433963	-1.4446180241
H	1.0	-0.9840784883	3.1499260896	-0.4327493320
H	1.0	-3.2153490654	3.0674717567	0.7493338447
H	1.0	-2.0006172326	1.9722364177	1.3836176783
H	1.0	-3.9692312028	0.9562417286	-0.7004011553
H	1.0	-4.4794612230	1.1228030102	0.9751884350
H	1.0	-3.8743638132	-1.1155439854	0.6827929838
H	1.0	-2.6768561697	-0.3964159126	1.7306884946
H	1.0	-0.0264841566	-1.2731340230	-2.0977238496
H	1.0	2.3896598115	-0.8459121077	-1.8956133153

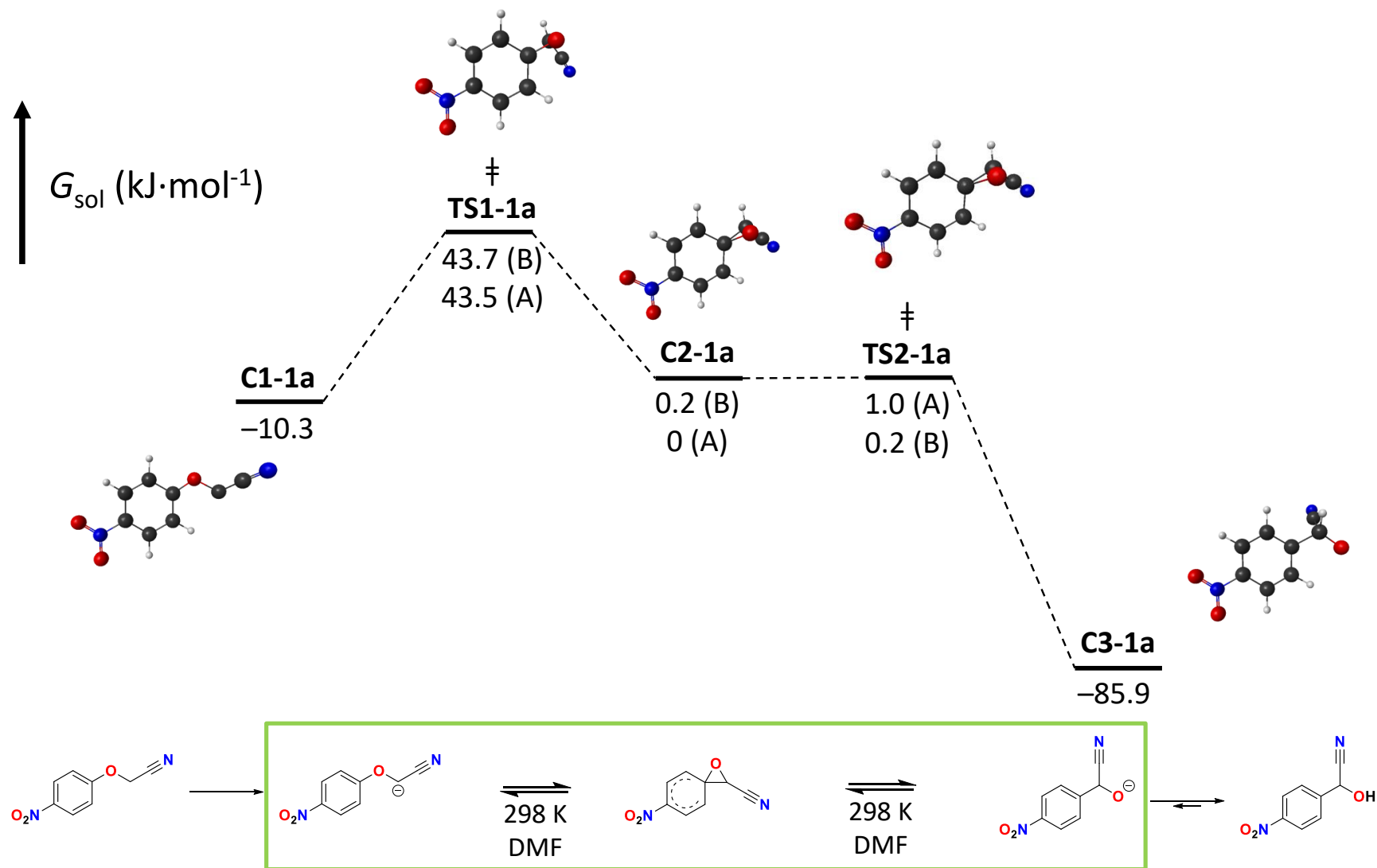
TS2-1e (conformer B – pseudo-axial)Energy: $-2100503.543 \text{ kJ mol}^{-1}$ Gibbs free energy: $-2099994.695 \text{ kJ mol}^{-1}$ Imaginary frequency: $146.76i \text{ cm}^{-1}$

C	6.0	-0.3987208301	-0.3858332316	0.4366556501
O	8.0	-1.1976869547	0.2772795824	-1.4558489039
C	6.0	-1.8766584465	1.4434297901	-1.6910128554
C	6.0	-2.5304061433	2.1014003156	-0.4627525340
C	6.0	-3.4402938304	1.1571379673	0.3295133045
C	6.0	-2.7639819990	0.2987262396	1.4012211580
C	6.0	-1.7786070612	-0.7993454535	0.9424153571
C	6.0	-2.4699763658	-1.7080244867	0.0168457804
N	7.0	-3.0897657546	-2.4766897301	-0.5912094239
C	6.0	0.2586752468	0.7239186390	1.0229442996
C	6.0	1.6090116610	0.9318827617	0.8475923618
C	6.0	2.3691012728	-0.0071185505	0.1379527065
C	6.0	1.7708016753	-1.1844458829	-0.3393560017
C	6.0	0.4237287023	-1.3815202952	-0.1568665368
N	7.0	3.7707395593	0.2010442915	-0.0403958829
O	8.0	4.2862342214	1.2288841458	0.4142823917
O	8.0	4.4290415903	-0.6503670919	-0.6488153071
H	1.0	-1.5811297247	-1.4168786706	1.8331586702
H	1.0	2.0870064475	1.8078975546	1.2706037755
H	1.0	-0.3038602440	1.4559840200	1.5886345447
H	1.0	-2.7057900261	1.2845361996	-2.4251487766
H	1.0	-1.2323264146	2.2280731053	-2.1583836496
H	1.0	-3.1214642174	2.9587085853	-0.8159154431
H	1.0	-1.7589830439	2.5137786041	0.2003195804
H	1.0	-3.9825237176	0.5067552052	-0.3707750883
H	1.0	-4.2051574452	1.7451352404	0.8515998408
H	1.0	-3.5452940713	-0.2128950614	1.9749330507
H	1.0	-2.2465903585	0.9405382420	2.1218984043
H	1.0	-0.0282746765	-2.2984462242	-0.5219201335
H	1.0	2.3769380088	-1.9367351941	-0.8305637805

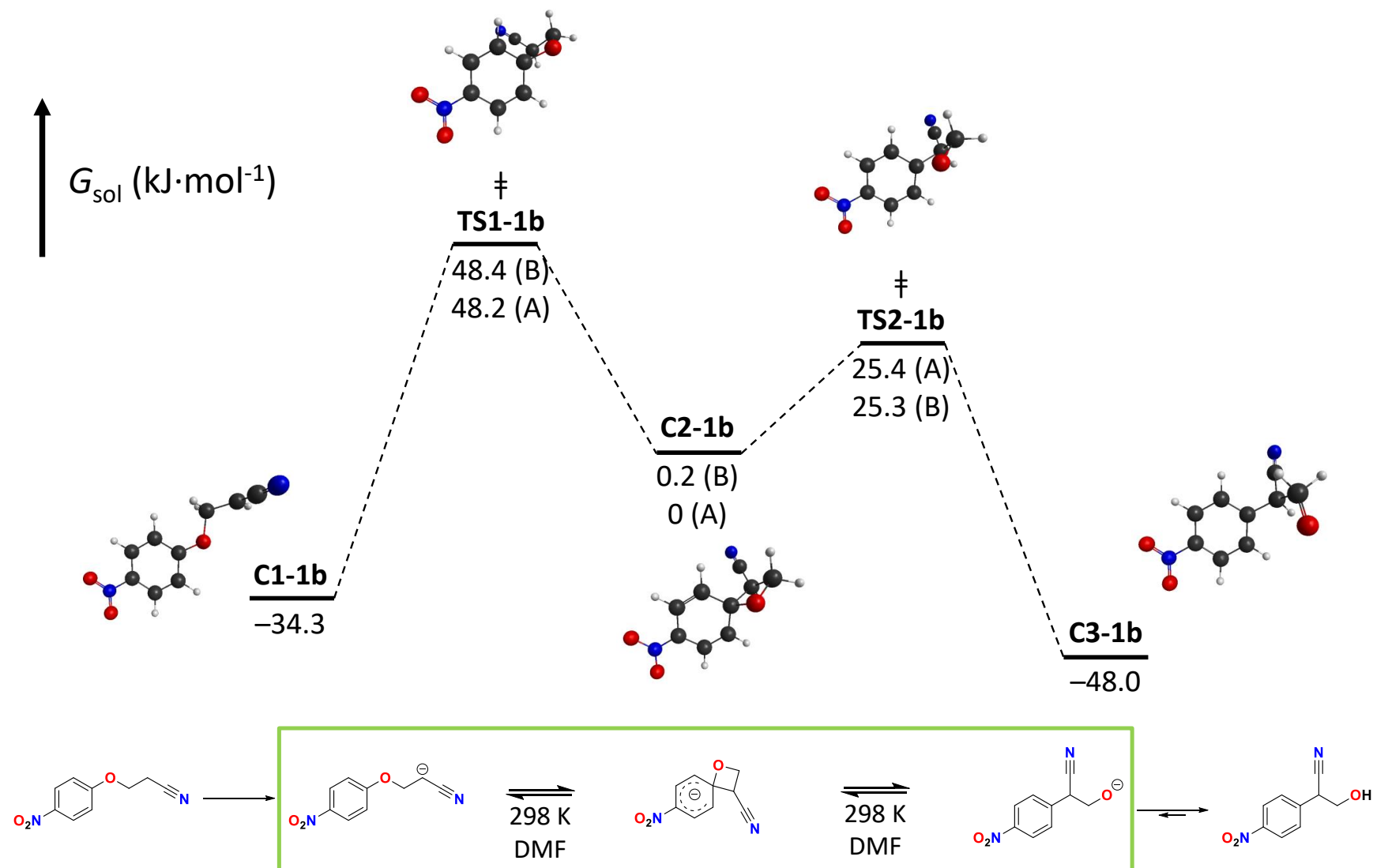
C3-1e**C3-1e**Energy: $-2100532.018 \text{ kJ mol}^{-1}$ Gibbs free energy: $-2100021.266 \text{ kJ mol}^{-1}$

C	6.0	-0.3353714045	-0.3472121084	1.0379395522
O	8.0	-1.5566410776	0.4255343943	-2.8729908644
C	6.0	-2.2543009488	1.5545285428	-2.5840029596
C	6.0	-2.3561785144	1.8636656039	-1.0700838473
C	6.0	-3.1310408388	0.7714693132	-0.3245107309
C	6.0	-2.7774081506	0.5937982089	1.1615829647
C	6.0	-1.7777266688	-0.5480313178	1.4981454045
C	6.0	-2.2825673458	-1.8358944571	0.9967407142
N	7.0	-2.6890744018	-2.8520268092	0.6160097546
C	6.0	0.6606102665	-0.2165595630	2.0117455196
C	6.0	1.9931005595	-0.0530853766	1.6543713725
C	6.0	2.3104915478	-0.0179956737	0.3019846151
C	6.0	1.3386920141	-0.1295467175	-0.6865327022
C	6.0	0.0102214741	-0.3021261825	-0.3184569457
N	7.0	3.7105392301	0.1439517970	-0.0920058066
O	8.0	4.5631392353	0.1583557332	0.7888175679
O	8.0	3.9686299556	0.2549375124	-1.2850404128
H	1.0	-1.7639336607	-0.6486920499	2.5898393440
H	1.0	2.7674735004	0.0395844052	2.4055476696
H	1.0	0.4017470141	-0.2496104315	3.0661148000
H	1.0	-3.3156019598	1.5319506789	-2.9626015356
H	1.0	-1.8229884036	2.4796539716	-3.0537621789
H	1.0	-2.8354255608	2.8410223678	-0.9063771182
H	1.0	-1.3362373561	1.9406731188	-0.6717565166
H	1.0	-2.9718707331	-0.1714262708	-0.8621827299
H	1.0	-4.2033022322	0.9850718613	-0.4019997264
H	1.0	-3.6813608943	0.3835047747	1.7428524345
H	1.0	-2.3537194266	1.5166698479	1.5743700756
H	1.0	-0.7298684005	-0.3313470066	-1.1282452981
H	1.0	1.6104921071	-0.0791126485	-1.7335798780

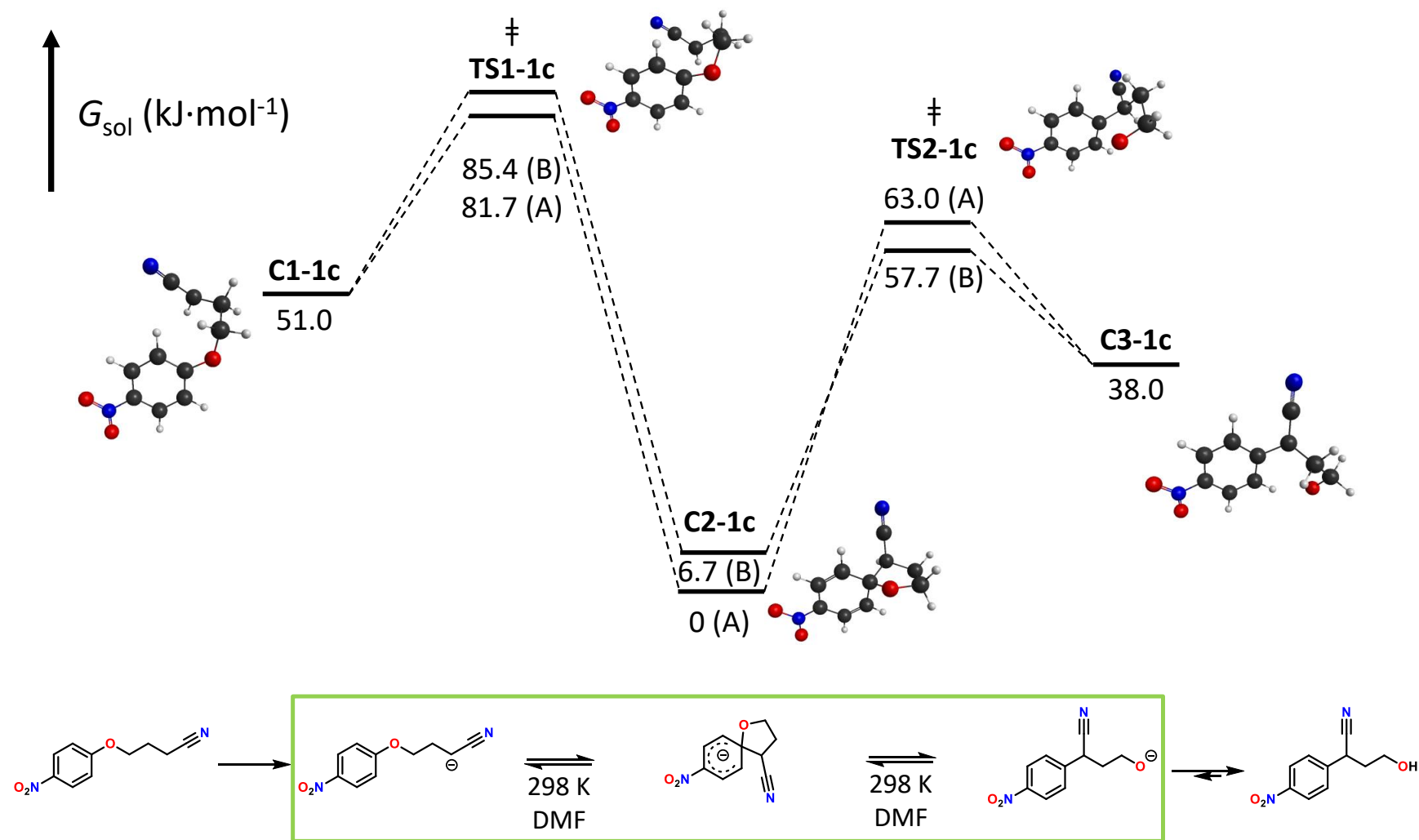
Calculated potential energy surface for pathway **1a** → **2a**



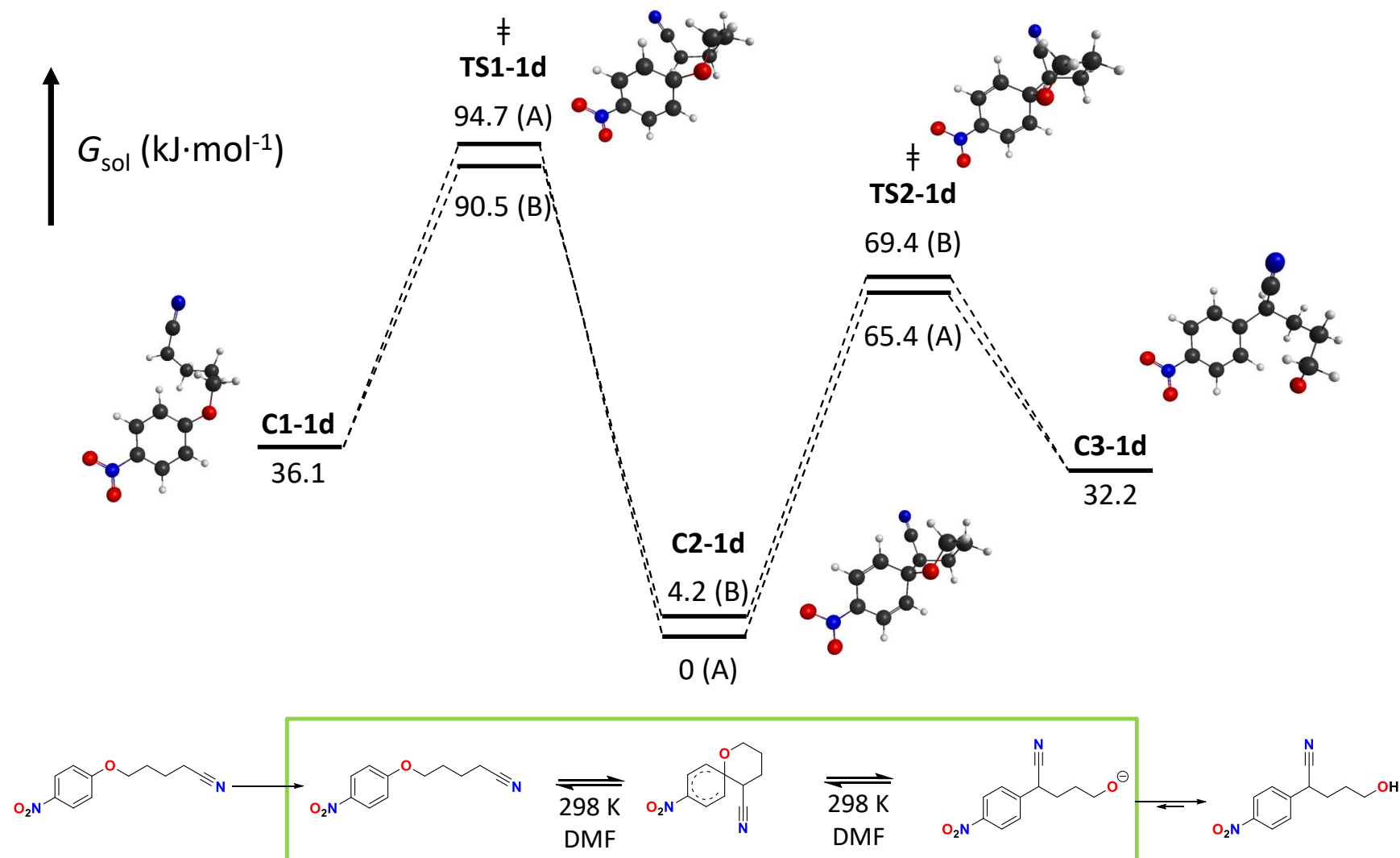
Calculated potential energy surface for pathway **1b** → **2b**



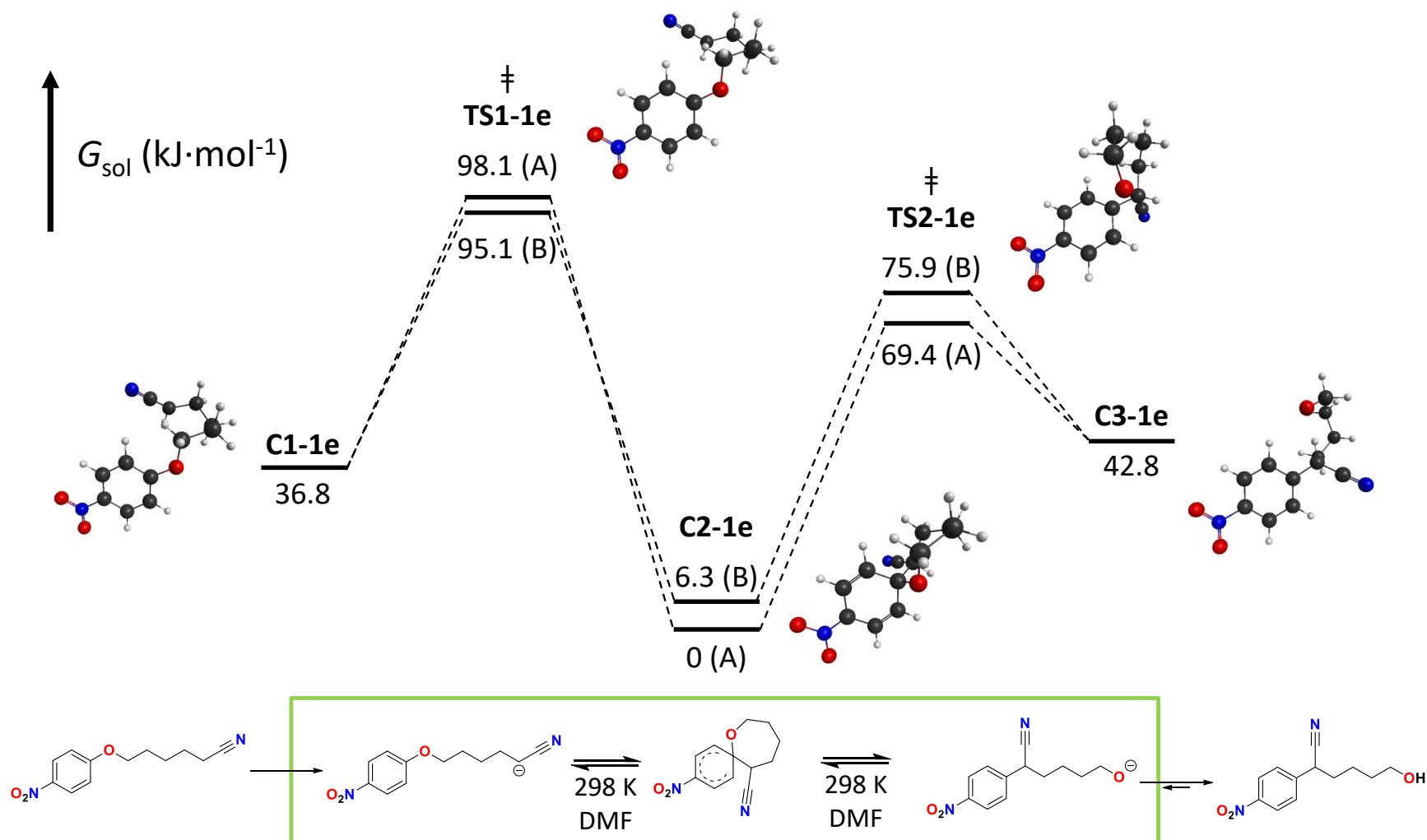
Calculated potential energy surface for pathway **1c** → **2c**



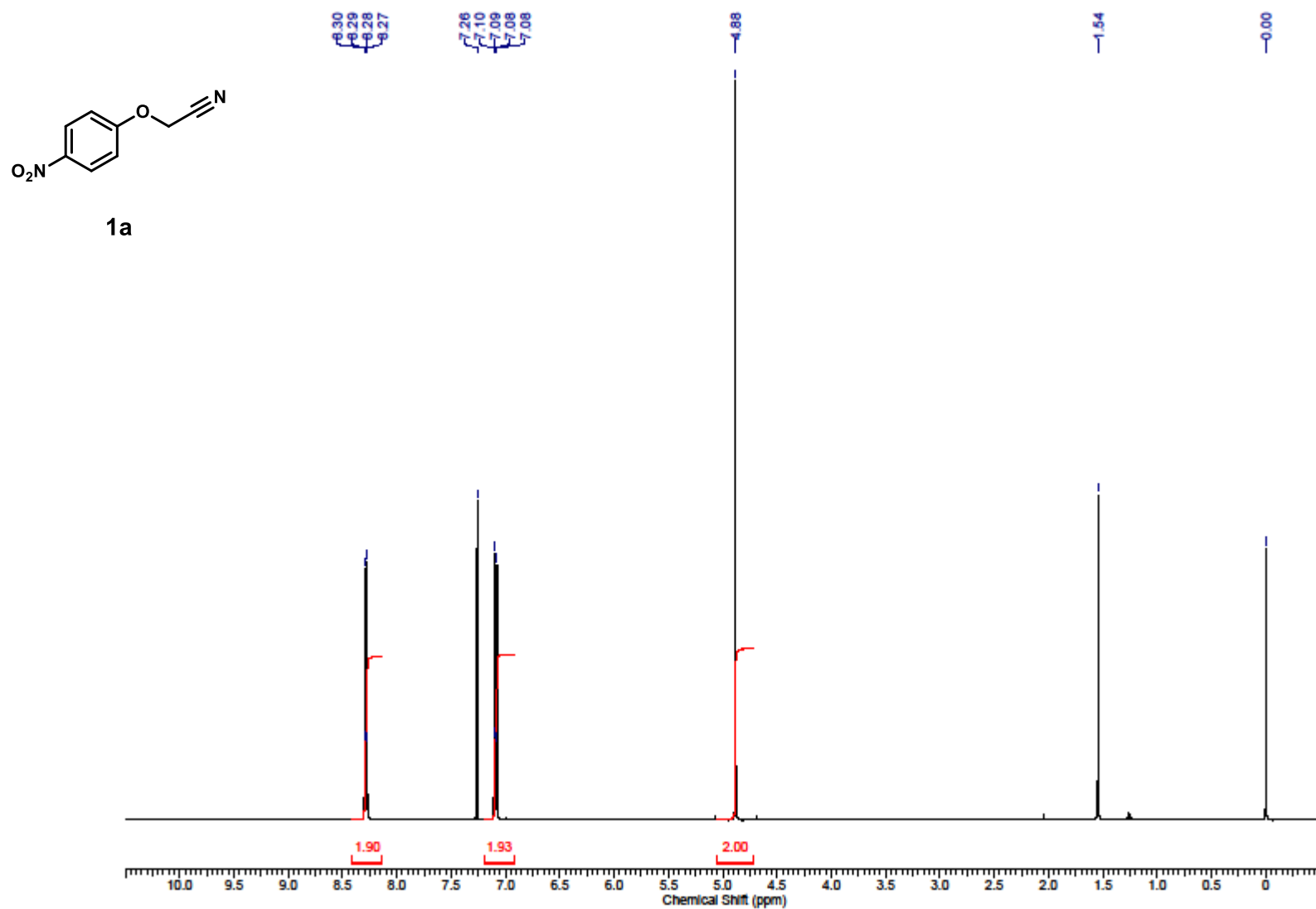
Calculated potential energy surface for pathway **1d** → **2d**



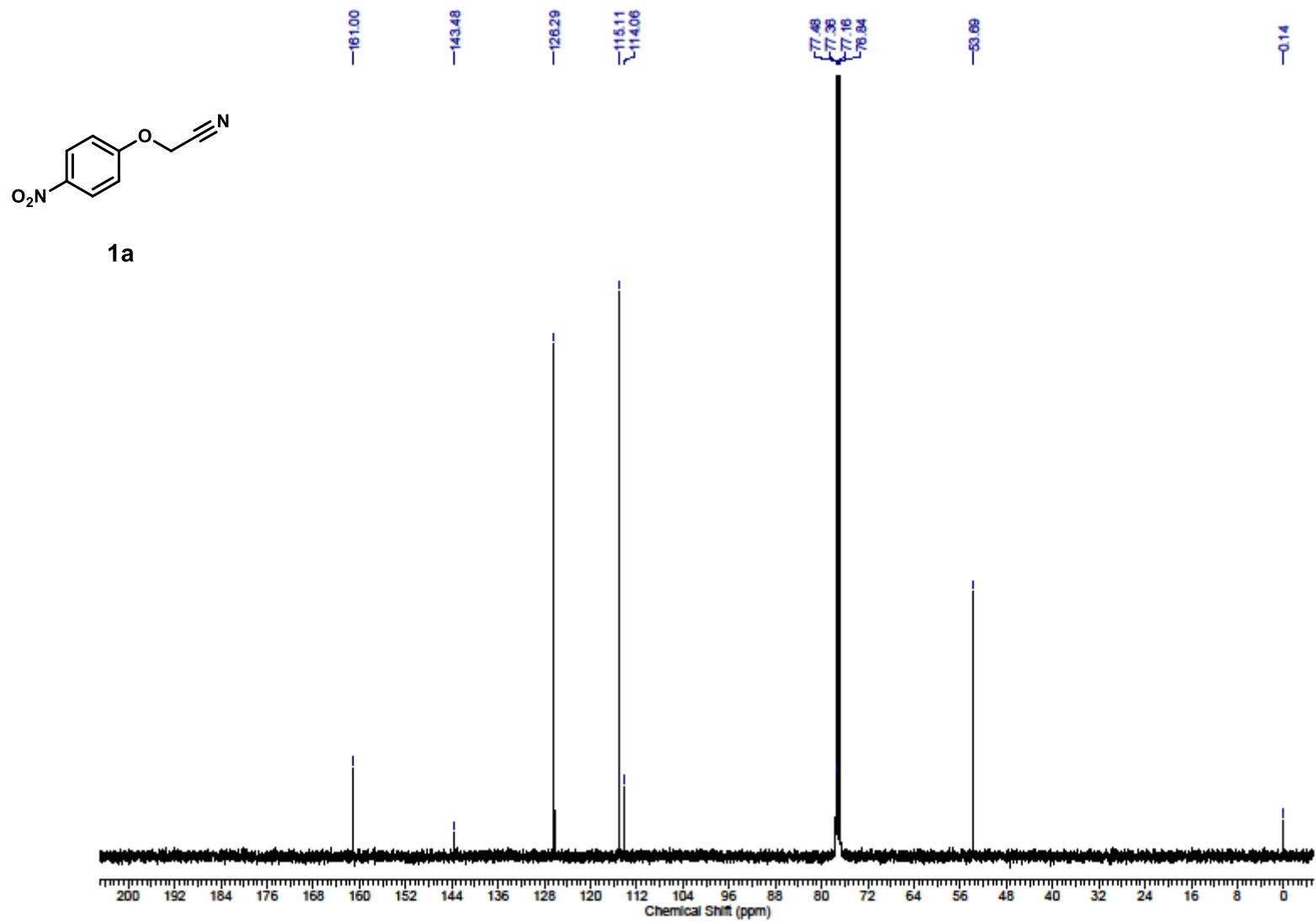
Calculated potential energy surface for pathway **1e** → **2e**



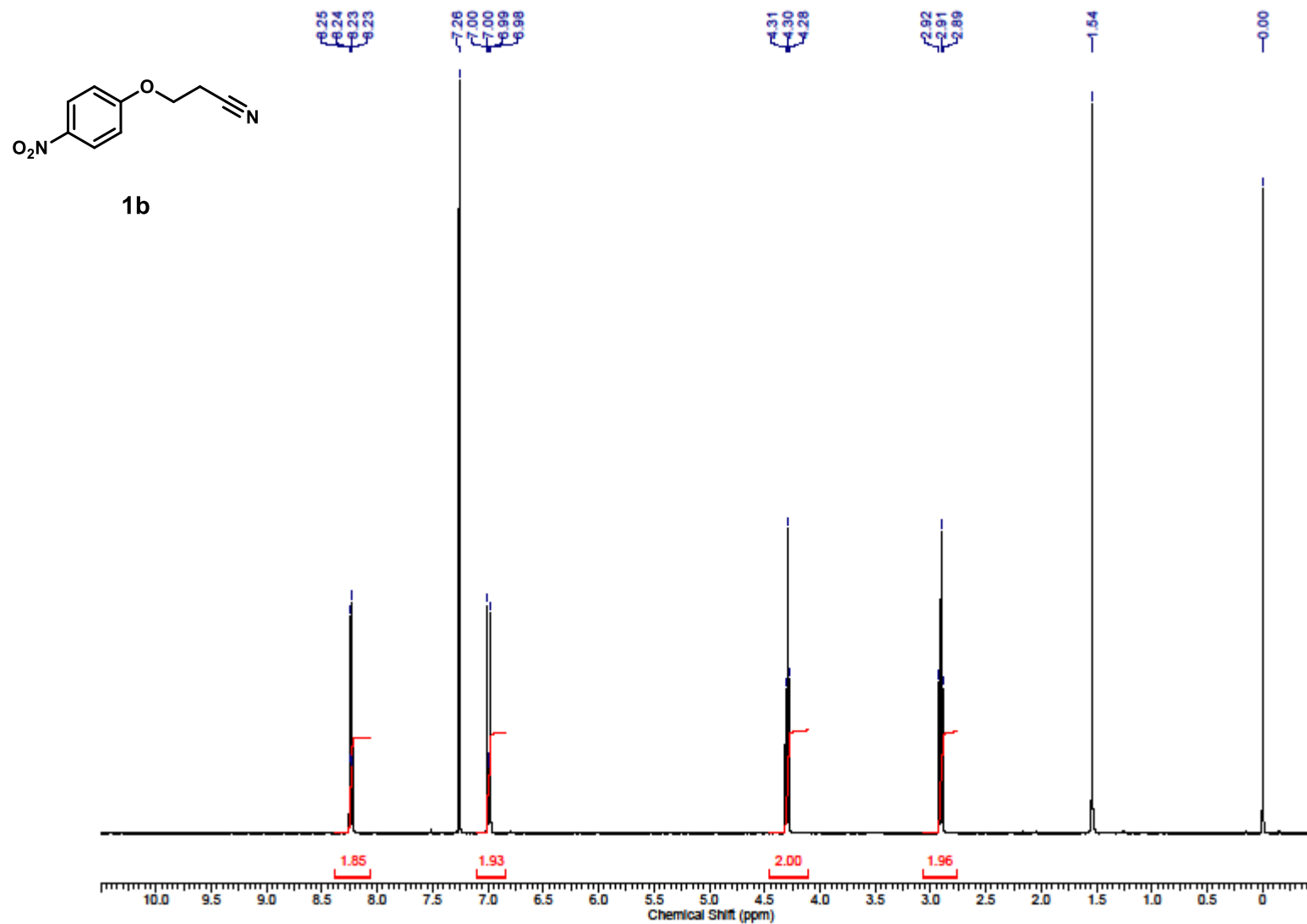
^1H NMR spectrum of **1a** in CDCl_3 with 0.05% v/v TMS (400 MHz)



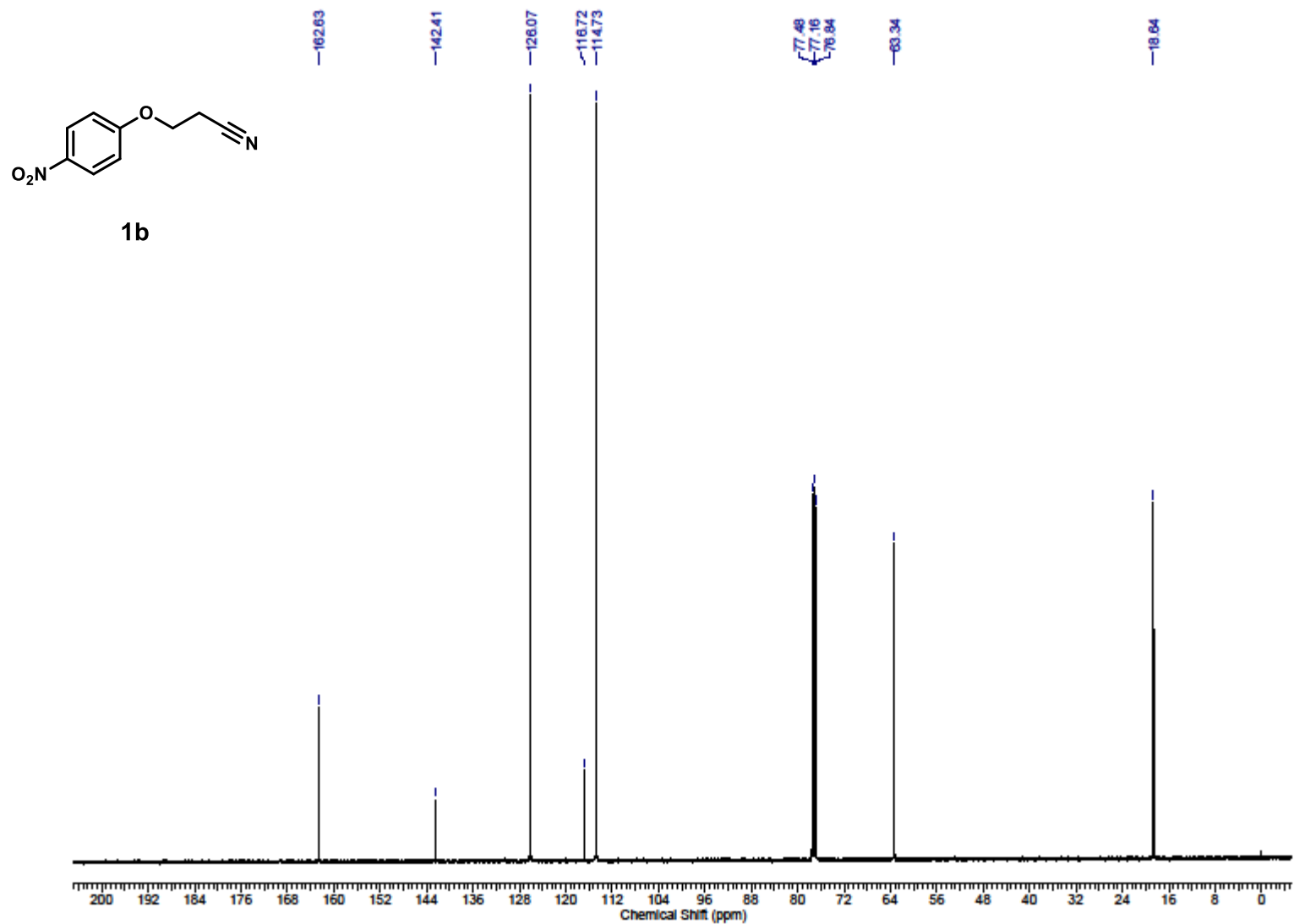
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1a** in CDCl_3 with 0.05% v/v TMS (100 MHz)



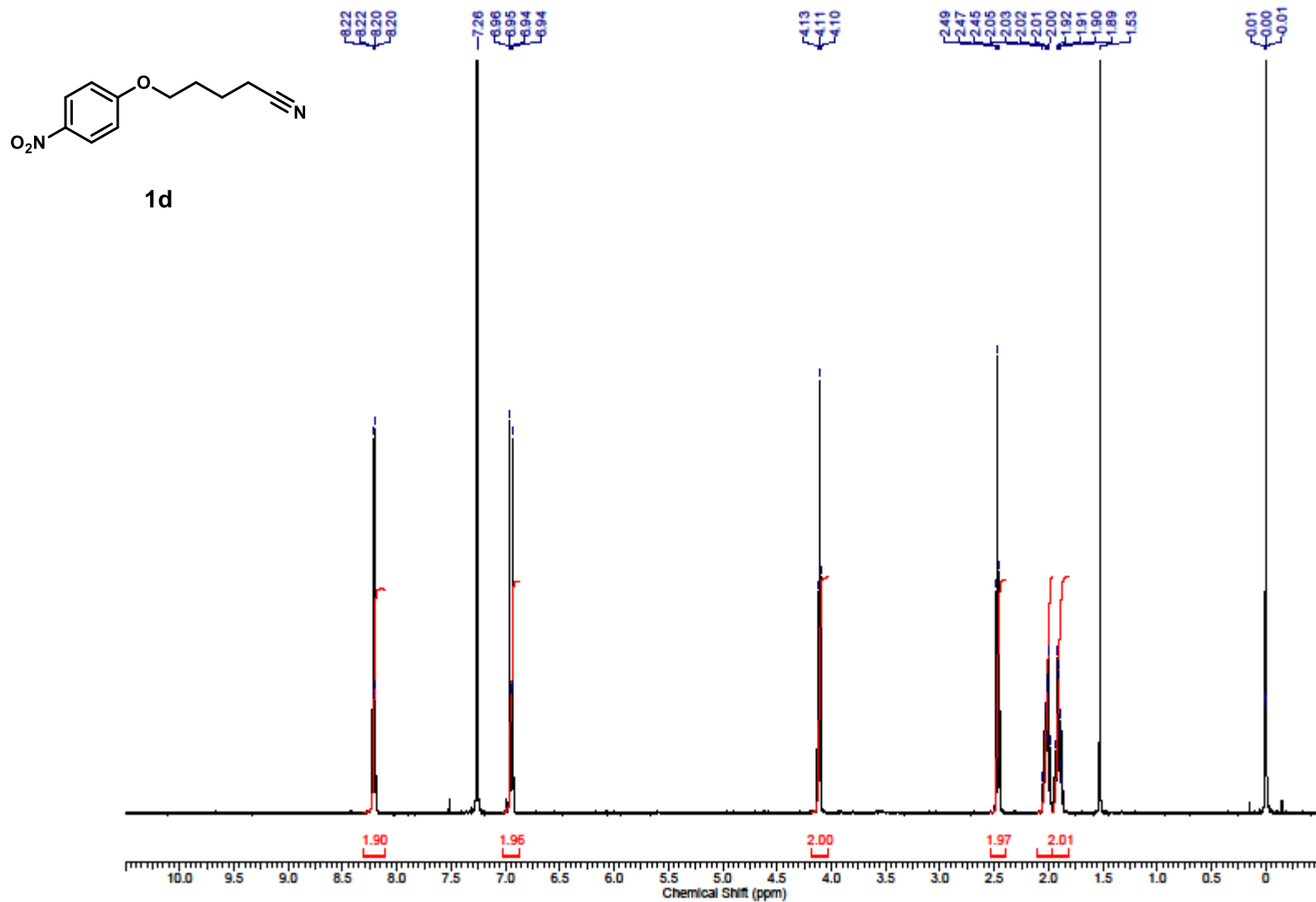
^1H NMR spectrum of **1b** in CDCl_3 with 0.05% v/v TMS (400 MHz)



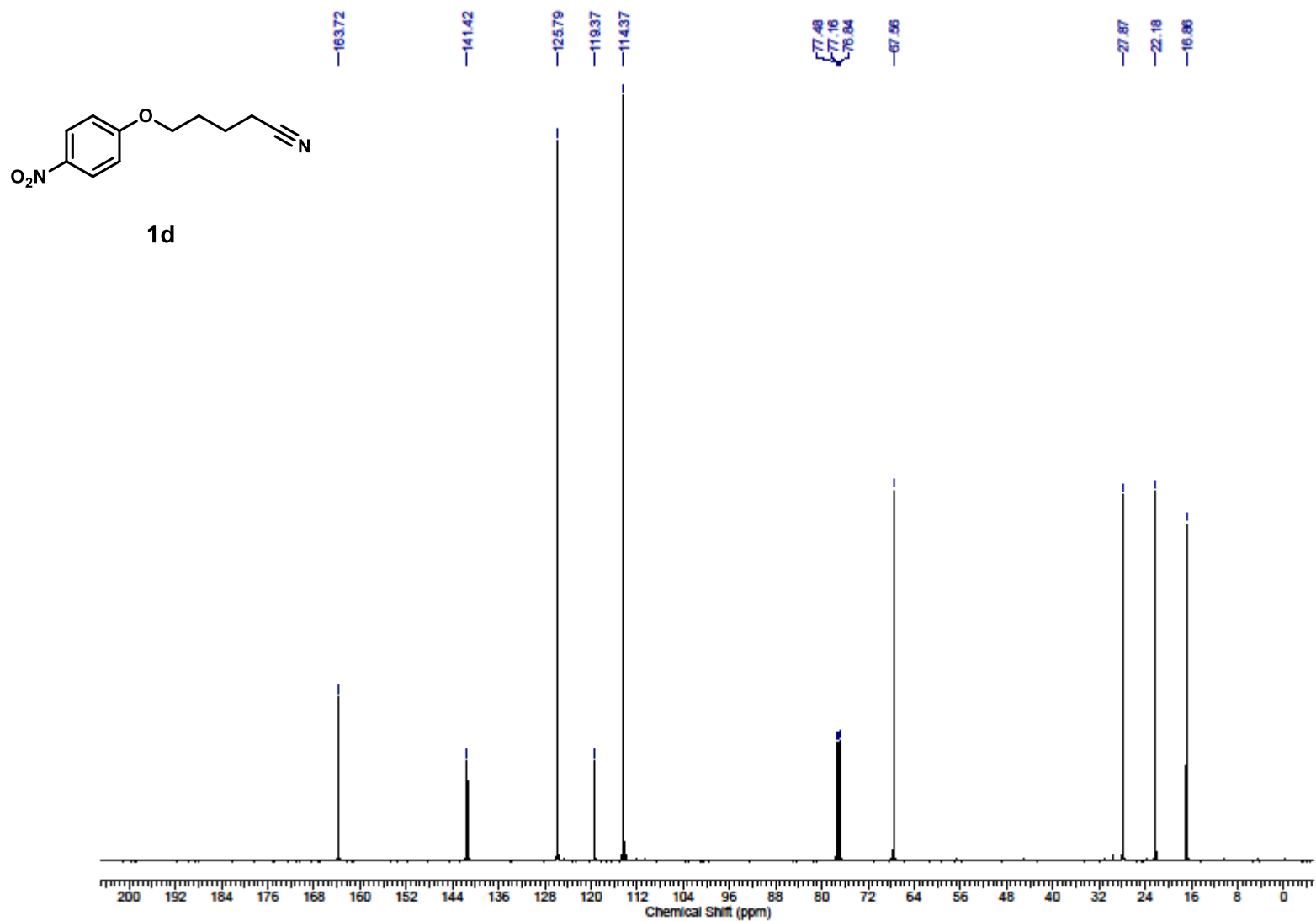
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1b** in CDCl_3 with 0.05% v/v TMS (100 MHz)



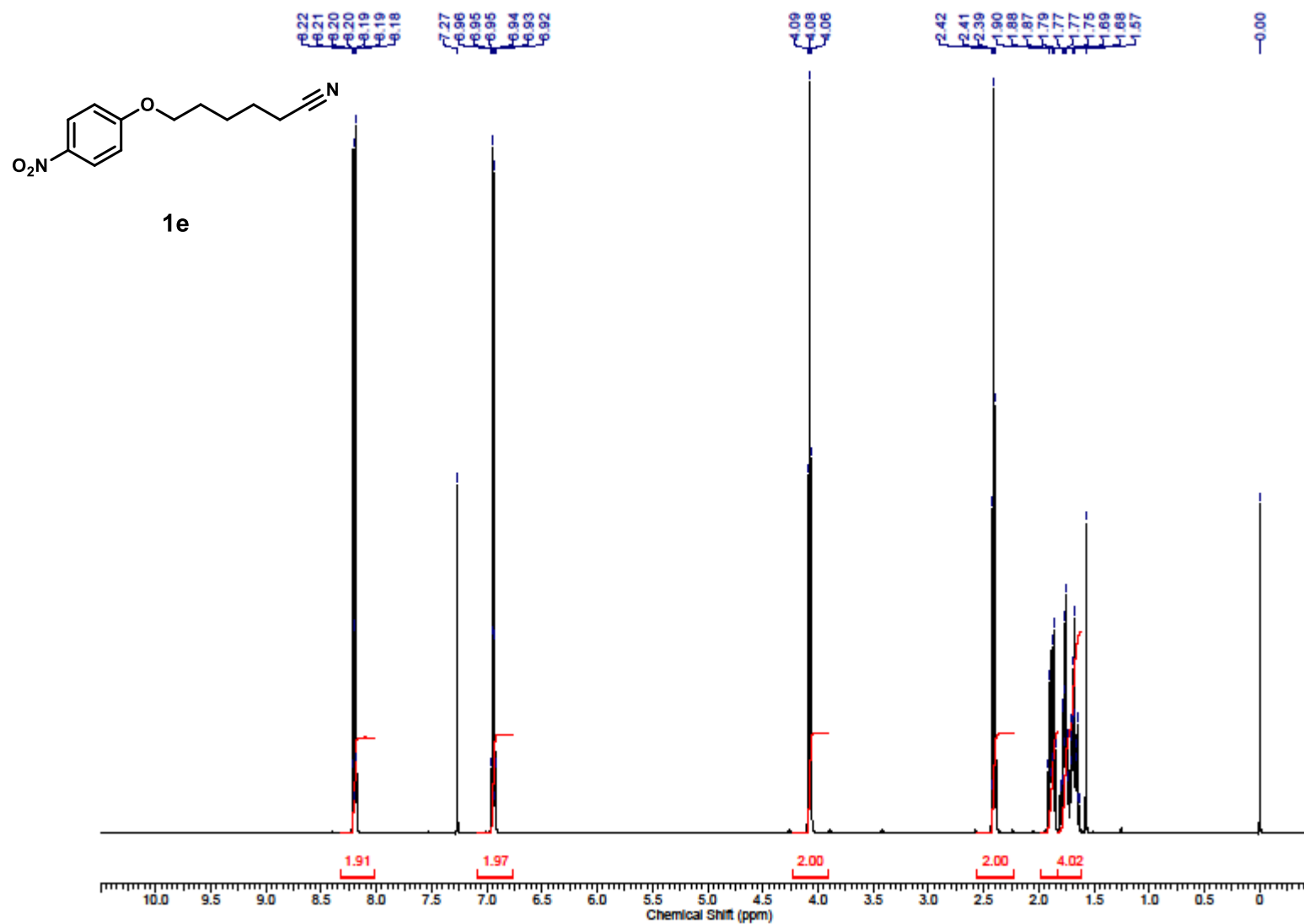
^1H NMR spectrum of **1d** in CDCl_3 with 0.05% v/v TMS (400 MHz)



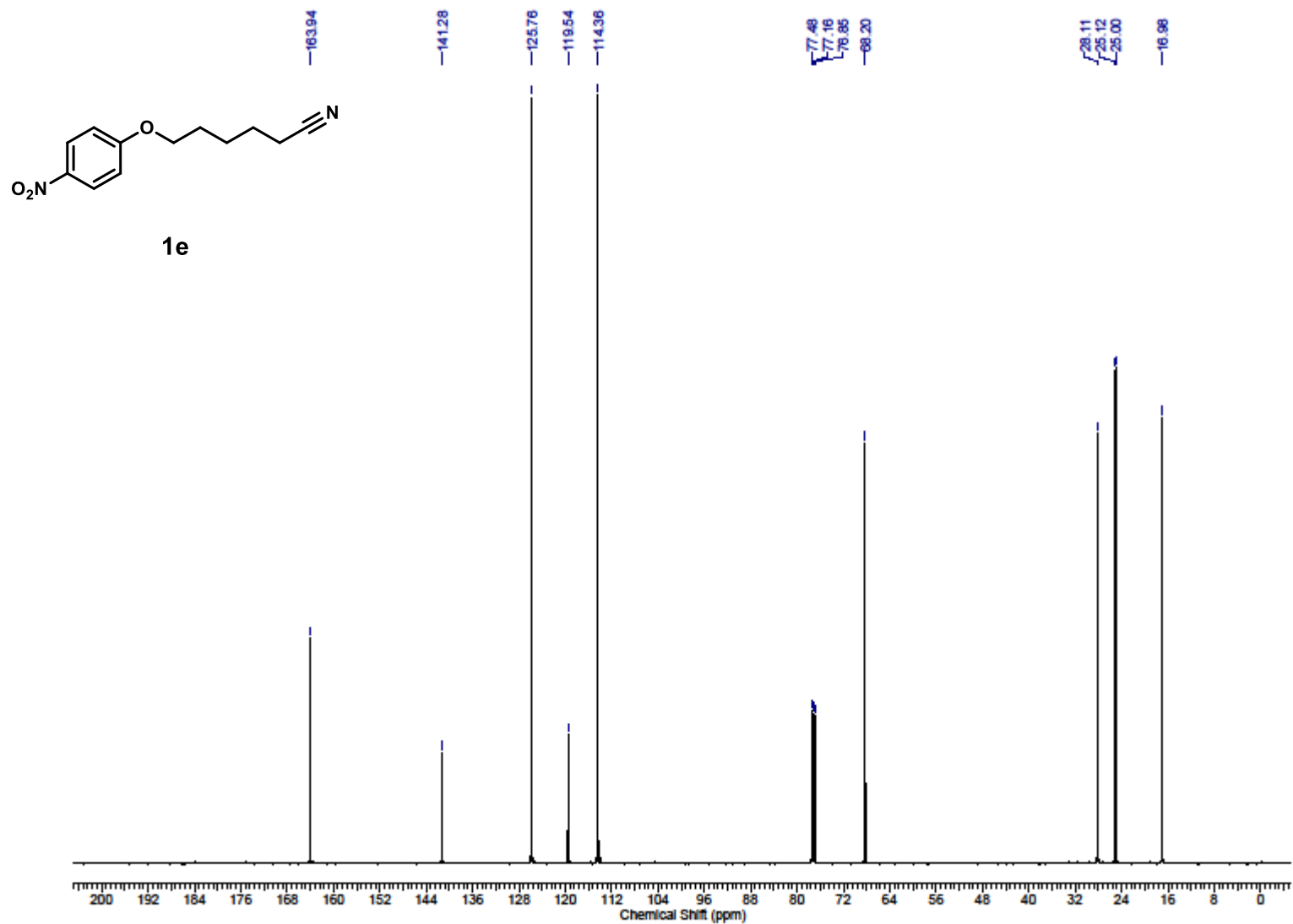
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1d** in CDCl_3 with 0.05% v/v TMS (100 MHz)



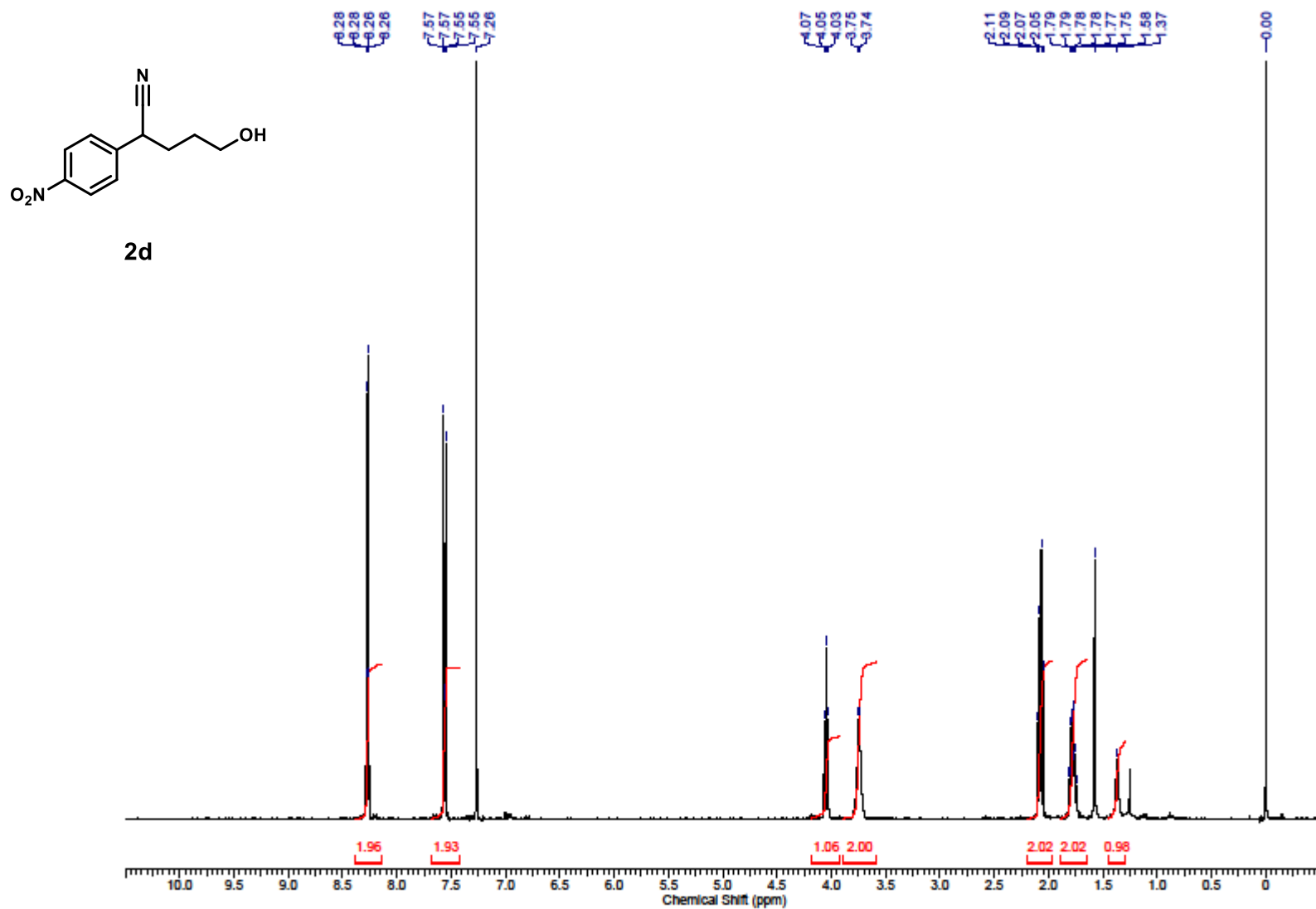
^1H NMR spectrum of **1e** in CDCl_3 with 0.05% v/v TMS (400 MHz)



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1e** in CDCl_3 with 0.05% v/v TMS (100 MHz)



^1H NMR spectrum of **2d** in CDCl_3 with 0.05% v/v TMS (400 MHz)



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2d** in CDCl_3 with 0.05% v/v TMS (100 MHz)

