Electronic Supplementary Information: Intrinsic defects and dopants in $LiNH_2$: A first-principles study

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TABLE I. Calculated formation energies for point defects and dopants in $LiNH_2$ at E_F=0.

Defect	E_f(eV)	Defect	E_f(eV)	Defect	E_f(eV)
Li_i^+	-1.98	Ti_{Li}^{3+}	-4.20	$(Sc_{Li}^+ + V_H)^0$	-1.49
Li_i^0	1.46	Ti_{Li}^{2+}	-2.66	Sc_{Li}^0	3.24
Li_i^-	4.99	$(Ti_{Li}^{2+} + V_H)^0$	-3.29	$(Sc_{Li}^0 + V_H)^0$	1.99
V_{Li}^+	2.92	Ti_{Li}^+	0.69	$(Sc_{Li}^0 + 2V_H)^0$	0.66
V_{Li}^0	2.95	$(Ti_{Li}^+ + V_H)^0$	-0.82	Ca_{Li}^+	-1.52
V_{Li}^-	3.12	$(Ti_{Li}^+ + 2V_H)^0$	-1.84	Ca_{Li}^0	1.95
H_i^+	-1.14	Ti_{Li}^0	3.71	$(Ca_{Li}^0 + V_H)^0$	1.12
H_i^0	2.34	$(Ti_{Li}^0 + V_H)^0$	2.39	Ca_{Li}^-	5.32
H_i^-	3.81	$(Ti_{Li}^0 + 2V_H)^0$	1.09	Mg_{Li}^+	-2.62
V_H^+	2.31	$(Ti_{Li}^0 + 3V_H)^0$	-0.06	Mg_{Li}^0	0.90
V_H^0	2.40	Sc_{Li}^{2+}	-3.43	$(Mg_{Li}^0 + V_H)^0$	0.08
V_H^-	3.24	Sc_{Li}^+	-0.15	Mg_{Li}^-	4.43

The calculated atomic coordinates in the cartesian mode (next pages), electronic energies E (eV) and thermal chemistry corrections (zero-point energy corrections, ZPE) of optimized structures in the proton transfer pathway (Fig. 3). All energies pertain to the full cell, i.e. $Li_{32}N_{32}H_{65}$.

(a) E= -614.274 eV, ZPE= 23.525 eV
(b) E= -613.826 eV, ZPE= 23.394 eV
(c) E= -614.237 eV, ZPE= 23.525 eV
(d) E= -613.632 eV, ZPE= 23.394 eV
(e) E= -614.274 eV, ZPE= 23.525 eV
Three lattice vectors are (in Å):

10.0263	0.0000	0.0000
0.0000	10.0263	0.0000
0.0000	0.0000	10.3428

TABLE II. The calculated atomic coordinates for local minimum (a). The coordinates of the hydrogen atom making a jump are boldface.

Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.
Li	10.01025	0.00625	-0.01814	N	1.40068	6.33460	6.36571	H	1.66315	7.96643	9.05237
Li	2.56535	2.45887	5.23454	N	3.69999	6.34406	3.96900	H	3.31753	7.10222	9.08870
Li	9.54253	2.10392	2.23576	N	1.25498	8.71998	3.96520	H	4.58976	9.18968	6.44279
Li	2.57625	-0.01351	7.76281	N	6.15822	6.25497	1.20787	H	0.49226	5.86411	6.45058
Li	10.00540	2.53941	10.26556	N	8.86625	8.80969	1.18986	H	4.26280	5.52055	3.72585
Li	2.53566	9.99418	10.25465	N	6.23351	8.87305	9.16488	H	0.80310	9.63713	3.87392
Li	2.53556	0.00303	5.21806	N	8.79180	6.18052	9.12504	H	6.15111	5.57446	1.97960
Li	9.86449	2.26698	5.32461	N	8.62787	8.72986	6.37055	H	8.85286	9.44139	2.00106
Li	5.01695	0.00767	0.01454	N	6.37194	6.27426	6.33739	H	5.56306	8.86863	8.38451
Li	7.46623	2.52752	5.22210	N	8.80481	6.34992	3.99215	H	9.46775	6.16116	8.35026
Li	5.03604	2.50856	2.58885	N	6.29376	8.65447	3.95865	H	8.62524	8.05174	7.14379
Li	7.48371	9.98619	7.78165	H	1.31497	0.57790	1.94192	H	6.37785	6.95019	7.11331
Li	5.02110	2.51367	0.07582	H	3.92948	4.46550	1.97675	H	8.22016	6.19266	3.16144
Li	7.50710	0.00806	10.27055	H	0.60446	3.89374	8.32594	H	6.98051	8.60576	3.19352
Li	7.43365	9.96953	5.30140	H	4.46225	1.17518	8.38502	H	7.06118	6.72691	1.33931
Li	5.02414	2.50560	5.10713	H	3.57230	3.11654	7.19458	H	7.94468	8.35929	1.24408
Li	10.01172	5.03130	-0.01300	H	1.32278	1.85099	7.20333	H	6.68399	7.95443	9.07697
Li	2.49191	7.58752	5.13268	H	3.17593	1.28389	3.15844	H	8.35919	7.10584	9.01771
Li	10.00558	7.55991	2.57833	H	2.13212	4.29682	3.40088	H	9.52735	9.20695	6.49757
Li	2.50077	5.06592	7.83872	H	1.97643	1.78510	1.10383	H	5.46679	5.80496	6.45820
Li	10.00867	7.53629	0.06550	H	2.97399	3.33874	1.34883	H	9.39298	5.50947	4.02767
Li	2.50333	5.01955	10.30914	H	1.73573	2.99332	9.01889	H	5.84944	9.56645	3.80007
Li	2.74075	5.20870	5.41910	H	3.32467	2.06414	9.08193	**H**	**1.47531**	**2.85855**	**3.01662**
Li	-0.00295	7.57251	5.10311	H	4.61165	4.11141	6.49840				
Li	5.00686	5.02697	10.34159	H	0.59089	0.60572	6.50153				
Li	7.52768	7.49209	5.13956	H	4.27565	0.46311	3.98562				
Li	5.03600	7.55599	2.56381	H	0.55554	4.03001	3.70780				
Li	7.49950	5.03983	7.74655	H	6.17007	0.55313	1.96866				
Li	5.00383	7.52847	0.07544	H	8.86096	4.36767	1.92803				
Li	7.48839	5.09262	10.23086	H	5.56926	3.87008	8.36707				
Li	7.53715	5.01286	5.22988	H	9.38782	1.13958	8.29345				
Li	5.02255	7.51628	5.09564	H	8.70007	3.16221	7.21719				
N	1.09070	1.28130	1.22627	H	6.39315	1.91100	7.18731				
N	3.88475	3.78790	1.20456	H	7.85718	1.32908	3.39383				
N	1.23311	3.88098	9.14054	H	6.94102	3.67159	3.19385				
N	3.78473	1.14964	9.15856	H	7.07777	1.70189	1.30740				
N	3.65553	3.75124	6.39030	H	7.82422	3.43717	1.13721				
N	1.35666	1.27370	6.35298	H	6.70894	2.98468	9.06710				
N	3.76056	1.35129	4.00087	H	8.27121	2.02986	9.02592				
N	1.47732	3.58465	3.75344	H	9.57355	4.24712	6.42409				
N	6.16498	1.24286	1.20560	H	5.41173	0.85141	6.49640				
N	8.81532	3.71024	1.13678	H	9.05910	0.38197	3.89041				
N	6.24633	3.89820	9.14035	H	5.83488	4.56991	3.93575				
N	8.78253	1.14482	9.12475	H	1.11610	5.66618	2.02031				
N	8.69962	3.71311	6.34776	H	3.86995	9.46403	2.00678				
N	6.34230	1.27085	6.38362	H	0.56790	8.91089	8.36466				
N	8.71352	1.34723	3.96686	H	4.43257	6.18587	8.39100				
N	6.29302	3.65332	3.99222	H	3.65134	8.07724	7.11943				
N	1.12760	6.26359	1.18538	H	1.38206	7.00258	7.14687				
N	3.85409	8.81111	1.21185	H	3.09395	6.46351	3.14623				
N	1.24277	8.89939	9.14046	H	1.90081	8.70905	3.16430				
N	3.76319	6.18087	9.17269	H	2.04152	6.72748	1.24954				
N	3.66554	8.75326	6.34414	H	2.94971	8.33808	1.32685				

TABLE III. The calculated atomic coordinates for local minimum (b). The coordinates of the hydrogen atom making a jump are boldface.

Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.
Li	9.98105	0.01883	0.07182	N	1.36963	6.34744	6.38392	H	1.54992	7.97755	9.09688
Li	2.51049	2.42509	5.13288	N	3.70161	6.36132	3.98115	H	3.27180	7.08922	9.06961
Li	9.43702	2.34415	2.42516	N	1.25922	8.71837	3.97482	H	4.58224	9.20250	6.43651
Li	2.54188	0.03844	7.69824	N	6.15165	6.25830	1.20239	H	0.44474	5.91408	6.48953
Li	9.92732	2.62211	10.33264	N	8.86331	8.82506	1.24161	H	4.21405	5.48828	3.80657
Li	2.75553	9.77247	10.12317	N	6.26360	8.88711	9.18972	H	0.79905	9.63334	3.90686
Li	2.52478	10.01886	5.21472	N	8.80982	6.21744	9.13211	H	6.13252	5.55985	1.95776
Li	10.00008	2.39452	5.09303	N	8.65370	8.74732	6.39437	H	8.82727	9.43974	2.06470
Li	5.09777	0.03483	0.03703	N	6.38765	6.25908	6.34924	H	5.61104	8.88345	8.39446
Li	7.50210	2.51470	5.24639	N	8.81922	6.35085	4.00492	H	9.49068	6.16928	8.36268
Li	5.04259	2.52614	2.60308	N	6.29820	8.63892	3.98643	H	8.66173	8.06122	7.16028
Li	7.52311	9.99765	7.79791	H	1.30937	0.61112	1.95732	H	6.37168	6.91125	7.14496
Li	5.03883	2.54212	0.08032	H	3.95308	4.51187	1.95527	H	8.20790	6.21940	3.18915
Li	7.53254	0.01590	10.30946	H	0.56273	3.90674	8.37459	H	6.99027	8.59832	3.22588
Li	7.45962	9.98652	5.31809	H	4.49038	1.16759	8.39506	H	7.05437	6.72341	1.35656
Li	5.02399	2.47634	5.11409	H	3.50982	3.10084	7.11963	H	7.95179	8.35362	1.27692
Li	10.00898	5.07842	10.35018	H	1.31612	1.93620	7.12702	H	6.71481	7.96810	9.11563
Li	2.50101	7.58269	5.15117	H	3.19169	1.25465	3.15442	H	8.37383	7.13474	8.98087
Li	10.02343	7.54587	2.61192	H	2.20076	3.64981	3.31516	H	9.56815	9.20291	6.49675
Li	2.47178	5.05964	7.80619	H	1.93920	1.73970	0.97793	H	5.49928	5.75517	6.45474
Li	9.97355	7.55031	0.10740	H	2.99941	3.35597	1.39042	H	9.39420	5.49925	4.01565
Li	2.50618	5.01409	10.30649	H	1.69500	2.98757	9.03565	H	5.85917	9.55469	3.83628
Li	2.61088	5.18756	5.34474	H	3.33171	2.03347	9.09002	**H**	**1.23422**	**2.35441**	**2.52318**
Li	0.00300	7.56806	5.11495	H	4.50656	4.13824	6.41246				
Li	5.00208	5.03563	10.32224	H	0.46739	0.75474	6.45279				
Li	7.53934	7.49253	5.17118	H	4.29153	0.42359	3.97694				
Li	5.04400	7.52947	2.59925	H	0.65893	4.03386	3.36175				
Li	7.55505	5.02244	7.72341	H	6.18951	0.60368	1.99726				
Li	5.01060	7.52957	0.07808	H	8.78392	4.51365	1.90264				
Li	7.47641	5.13641	10.20426	H	5.59798	3.89393	8.33418				
Li	7.56701	5.00465	5.22940	H	9.44561	1.15499	8.37822				
Li	5.02667	7.49781	5.11803	H	8.79262	3.10670	7.15577				
N	1.09775	1.51839	1.52259	H	6.38801	1.93683	7.21507				
N	3.90234	3.80554	1.20908	H	7.80031	1.21785	3.38378				
N	1.20563	3.87969	9.17829	H	6.94043	3.65941	3.22118				
N	3.81040	1.12841	9.16499	H	7.10070	1.73455	1.31033				
N	3.56206	3.74420	6.31974	H	7.75936	3.53706	1.14752				
N	1.35297	1.26428	6.34910	H	6.72239	3.00286	9.05302				
N	3.78711	1.31727	3.98896	H	8.28570	2.02718	9.06436				
N	1.28707	3.24370	3.56334	H	9.64287	4.22478	6.38325				
N	6.19189	1.26808	1.21163	H	5.43602	0.83565	6.54703				
N	8.75290	3.80046	1.16078	H	9.08534	0.40169	3.89789				
N	6.25195	3.91217	9.12767	H	5.83932	4.56794	3.95725				
N	8.83136	1.16824	9.20280	H	1.22142	5.68039	2.01635				
N	8.74387	3.73045	6.33905	H	3.96671	9.50490	1.98852				
N	6.35667	1.27501	6.42811	H	0.57614	9.05794	8.42850				
N	8.63528	1.32178	3.97746	H	4.41086	6.20275	8.37103				
N	6.29353	3.64933	4.02099	H	3.65911	8.09815	7.14656				
N	1.13842	6.28862	1.19243	H	1.38821	7.03074	7.15152				
N	3.87945	8.82304	1.22290	H	3.06557	6.41536	3.17412				
N	1.22745	8.94642	9.21557	H	1.90737	8.72942	3.17646				
N	3.75229	6.18620	9.16173	H	2.03916	6.78119	1.18373				
N	3.65703	8.76365	6.36235	H	3.01167	8.32940	1.46515				

TABLE IV. The calculated atomic coordinates for local minimum (c). The coordinates of the hydrogen atoms making a jump are boldface.

Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.
Li	10.01617	9.98590	10.23514	N	1.39662	6.31317	6.35819	H	1.57220	7.86222	8.96955
Li	2.50328	2.52758	5.21895	N	3.74961	6.36862	3.95383	H	3.33140	7.08986	9.06070
Li	9.62981	2.91640	2.95435	N	1.26651	8.69708	3.96475	H	4.60540	9.18542	6.43079
Li	2.54989	9.99501	7.68575	N	6.17878	6.23953	1.20914	H	0.48399	5.85751	6.47338
Li	9.66890	2.77718	9.98204	N	8.91651	8.83447	1.18262	H	4.21667	5.46032	3.84600
Li	2.66673	9.72803	10.10425	N	6.25198	8.85782	9.17262	H	0.78305	9.60279	3.95180
Li	2.54027	0.01746	5.22555	N	8.78238	6.19937	9.14860	H	6.17613	5.58525	2.00316
Li	0.00366	2.51543	5.27865	N	8.66091	8.73498	6.35053	H	8.90872	9.45671	2.00100
Li	5.07229	0.00734	0.03510	N	6.36706	6.30518	6.35047	H	5.55957	8.87534	8.41137
Li	7.50404	2.53231	5.24931	N	8.76242	6.38183	3.94869	H	9.42070	6.15002	8.34338
Li	5.03790	2.52610	2.60596	N	6.28982	8.68656	3.96044	H	8.69502	8.05301	7.12007
Li	7.47903	9.90368	7.72802	**H**	**1.07247**	**0.62427**	**2.07682**	H	6.37130	6.98927	7.11887
Li	5.01459	2.51175	0.07555	H	3.83483	4.40808	1.99680	H	8.07570	6.39415	3.18295
Li	7.53901	9.98933	10.29095	H	0.72816	3.90580	8.20944	H	6.94053	8.71838	3.16447
Li	7.50608	0.00298	5.24714	H	4.45420	1.12720	8.38719	H	7.07390	6.72969	1.32417
Li	5.01137	2.51159	5.12411	H	3.64511	3.10156	7.18776	H	8.02222	8.33750	1.27662
Li	0.04975	5.10757	10.29173	H	1.35381	1.86062	7.22384	H	6.67034	7.92504	9.07463
Li	2.51870	7.53746	5.13074	H	3.08215	1.45804	3.20507	H	8.36545	7.13180	9.04200
Li	0.02033	7.53629	2.58349	H	1.84997	3.66923	3.26175	H	9.56869	9.20710	6.43164
Li	2.55872	5.08394	7.75527	H	2.34916	1.22211	1.25443	H	5.44578	5.86217	6.44962
Li	0.00063	7.53772	0.06956	H	2.93246	3.28916	1.29376	H	9.21622	5.46869	3.82830
Li	2.52795	5.01948	10.27604	H	1.73785	3.02019	9.08805	H	5.80518	9.58933	3.89269
Li	2.56965	5.05257	5.27117	H	3.27629	1.96476	9.08588	**H**	**0.95724**	**2.06412**	**1.29821**
Li	10.02579	7.51734	5.08610	H	4.59399	4.18414	6.48230				
Li	5.00041	5.01315	0.02958	H	0.49073	0.73287	6.47696				
Li	7.51758	7.53026	5.14203	H	4.16465	0.46667	3.85253				
Li	5.04840	7.50334	2.60238	H	0.87997	4.67109	4.05127				
Li	7.47348	5.06043	7.74014	H	6.22786	0.61506	1.99874				
Li	5.01589	7.50870	0.09017	H	8.95926	4.63187	1.76966				
Li	7.46950	5.10009	10.22829	H	5.58209	3.86467	8.36584				
Li	7.52801	5.03873	5.24421	H	9.34134	1.13110	8.24372				
Li	5.02012	7.52122	5.08544	H	8.70459	3.19694	7.25873				
N	1.32904	1.11060	1.20977	H	6.36660	1.92153	7.19030				
N	3.83982	3.75832	1.19890	H	8.04160	1.28262	3.25982				
N	1.19679	3.89234	9.12552	H	6.93564	3.65713	3.20326				
N	3.78860	1.07932	9.16975	H	7.10876	1.72847	1.25360				
N	3.66389	3.75731	6.39562	H	7.96092	3.45371	1.32134				
N	1.36905	1.25821	6.38999	H	6.72472	3.00117	9.09225				
N	3.73894	1.39102	3.99129	H	8.03616	1.79926	8.89698				
N	1.18949	3.69063	4.05123	H	9.54266	4.30601	6.45515				
N	6.19833	1.25775	1.19561	H	5.43985	0.82434	6.48335				
N	8.92908	3.77722	1.19426	H	9.28530	0.55926	3.96797				
N	6.22965	3.89668	9.16401	H	5.84936	4.58274	3.93379				
N	8.79570	1.14268	9.11549	H	1.20796	5.63558	1.98861				
N	8.66591	3.77352	6.40825	H	3.99382	9.46309	1.99259				
N	6.37086	1.25187	6.40943	H	0.58506	8.92347	8.29727				
N	8.72991	1.42106	4.01224	H	4.47445	6.17294	8.40552				
N	6.29366	3.65951	4.00647	H	3.66573	8.07259	7.10191				
N	1.16112	6.26833	1.17946	H	1.39161	7.01510	7.10958				
N	3.86644	8.80426	1.21236	H	3.08759	6.37267	3.16635				
N	1.23388	8.82497	9.08850	H	1.91820	8.76531	3.17264				
N	3.78865	6.17720	9.17266	H	2.07120	6.74167	1.20587				
N	3.67682	8.75757	6.33415	H	3.00586	8.31113	1.47840				

TABLE V. The calculated atomic coordinates for local minimum (d). The coordinates of the hydrogen atom making a jump are boldface.

Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.
Li	0.02487	9.91385	0.02599	N	1.41969	6.37560	6.30898	H	1.71876	7.95232	8.99047
Li	2.54181	2.57741	5.20142	N	3.78501	6.40652	3.94666	H	3.39506	7.11230	9.10410
Li	9.74273	2.94075	2.90626	N	1.42743	8.99988	3.65581	H	4.51257	9.32444	6.38009
Li	2.51170	0.01746	7.73871	N	6.21641	6.20873	1.20628	H	0.67323	5.70507	6.53074
Li	9.97563	2.64350	10.24210	N	8.79320	8.67792	1.12092	H	4.29159	5.51363	3.91694
Li	2.55084	9.90156	10.31787	N	6.28367	8.92240	9.11082	H	0.41798	8.91911	3.84267
Li	2.47738	0.09040	5.15123	N	8.75750	6.15619	9.09936	H	6.12941	5.52735	1.97219
Li	0.03426	2.62613	5.26941	N	8.70636	8.75649	6.36025	H	8.77638	9.28982	1.94797
Li	5.04923	-0.00641	0.01321	N	6.32889	6.33467	6.35744	H	5.58466	8.94299	8.35616
Li	7.54918	2.56317	5.18529	N	8.75081	6.40674	3.96741	H	9.33429	6.16174	8.24846
Li	5.03885	2.51749	2.59962	N	6.34421	8.72391	3.97035	H	8.70846	8.20214	7.22741
Li	7.52620	10.04861	7.73756	H	0.34359	1.06383	1.89585	H	6.34450	6.98928	7.15067
Li	5.03045	2.48892	0.08785	H	3.69887	4.31099	2.02805	H	7.92592	6.41422	3.35128
Li	7.53190	0.03351	10.25976	H	0.67242	3.85629	8.26653	H	6.98674	8.71879	3.16729
Li	7.57465	0.06425	5.22623	H	4.42740	1.12927	8.39893	H	7.14071	6.62213	1.37798
Li	5.05170	2.57578	5.10914	H	3.66351	3.10126	7.14957	H	7.82879	8.32702	1.08094
Li	0.01745	5.05399	10.24550	H	1.38615	1.92259	7.20655	H	6.72270	8.00362	8.98076
Li	2.57017	7.57902	5.10184	H	3.13777	1.37142	3.22430	H	8.27589	7.06158	9.04952
Li	9.72046	7.25142	2.31612	H	1.88720	3.70572	3.25221	H	9.60181	9.25718	6.41314
Li	2.62705	5.07618	7.77734	H	1.90255	1.43426	1.72049	H	5.38781	5.92890	6.42329
Li	9.99748	7.49932	10.26609	H	2.96632	3.16204	1.16911	H	9.11170	5.45027	3.85970
Li	2.52744	5.02903	10.28045	H	1.81521	3.03100	9.02400	H	5.84752	9.61496	3.85603
Li	2.62189	5.08594	5.24550	H	3.31948	2.03350	9.11973	**H**	**1.40905**	**-0.16745**	**2.63377**
Li	9.85898	7.31052	5.34170	H	4.64148	4.20323	6.51748				
Li	5.00416	4.99255	0.04407	H	0.44865	0.85849	6.46001				
Li	7.47158	7.59552	5.20813	H	4.25071	0.52238	3.99291				
Li	5.09888	7.53879	2.57183	H	0.93548	4.76269	3.99360				
Li	7.41683	5.02546	7.75175	H	6.17203	0.58738	1.98690				
Li	5.10028	7.51335	0.07352	H	8.88978	4.60539	1.79608				
Li	7.47744	5.03196	10.22034	H	5.52866	3.83667	8.39506				
Li	7.44827	5.03262	5.27243	H	9.50243	1.13022	8.38932				
Li	5.02586	7.60051	5.07323	H	8.67295	3.19928	7.22776				
N	1.23968	0.66029	1.58508	H	6.41563	2.00118	7.14891				
N	3.81415	3.74340	1.17852	H	8.18340	1.21854	3.23015				
N	1.25827	3.88977	9.11163	H	6.98184	3.63075	3.17435				
N	3.76739	1.11256	9.18882	H	7.11131	1.71002	1.33190				
N	3.70262	3.80376	6.39837	H	8.00429	3.37814	1.24955				
N	1.35697	1.32993	6.36644	H	6.68543	2.94498	9.05880				
N	3.79185	1.44111	4.01203	H	8.32669	2.00429	9.05038				
N	1.23606	3.78099	4.04676	H	9.47923	4.38330	6.49857				
N	6.20436	1.24758	1.19866	H	5.51338	0.86754	6.46512				
N	8.94778	3.77974	1.18319	H	9.51061	0.71355	3.99503				
N	6.22182	3.85629	9.15449	H	5.87264	4.60620	3.79511				
N	8.89233	1.16179	9.21678	H	1.27204	5.58100	1.92270				
N	8.63678	3.80634	6.39890	H	3.94994	9.43669	1.98798				
N	6.43084	1.32038	6.37762	H	0.61172	8.89291	8.30953				
N	8.80750	1.46024	4.01109	H	4.50415	6.18257	8.41125				
N	6.32746	3.70127	3.96480	H	3.67253	8.15144	7.08673				
N	1.09739	6.25023	1.16199	H	1.42882	6.99190	7.13218				
N	3.96646	8.76470	1.20904	H	3.21329	6.36181	3.09317				
N	1.23055	8.84529	9.12938	H	1.66042	8.14934	3.12324				
N	3.81855	6.17974	9.17871	H	1.94592	6.82752	1.15544				
N	3.62853	8.80945	6.29674	H	3.08314	8.26259	1.35059				

TABLE VI. The calculated atomic coordinates for local minimum (e). The coordinates of the hydrogen atom making a jump are boldface.

Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.	Atom	x-coord.	y-coord.	z-coord.
Li	10.02017	0.02143	10.32034	N	1.36615	6.30458	6.36890	H	1.75916	8.00781	9.04534
Li	2.49494	2.57582	5.14573	N	3.75413	6.37400	4.00342	H	3.34816	7.08348	9.08515
Li	10.00655	2.55180	2.57725	N	1.51156	8.69211	3.81321	H	4.65133	9.10940	6.52570
Li	2.52800	0.04910	7.84392	N	6.17399	6.25873	1.22065	H	0.62290	5.61870	6.54862
Li	10.01803	2.52862	0.06295	N	8.83071	8.73373	1.14331	H	4.25116	5.47645	3.95934
Li	2.51060	0.01841	10.31466	N	6.24801	8.91805	9.15272	H	0.55630	9.06013	3.84354
Li	2.78042	0.18826	5.42272	N	8.78905	6.17067	9.13510	H	6.16863	5.56744	1.98235
Li	10.02415	2.53986	5.10539	N	8.68410	8.73401	6.36212	H	8.86922	9.39984	1.92748
Li	5.01255	0.01892	0.02153	N	6.35315	6.28944	6.38997	H	5.55659	8.89813	8.39193
Li	7.52684	2.49643	5.16260	N	8.72575	6.37812	3.97974	H	9.38877	6.18180	8.29992
Li	5.05882	2.57034	2.56790	N	6.28533	8.67537	4.00019	H	8.66797	8.19766	7.24054
Li	7.48422	0.04213	7.75751	H	1.08901	0.63789	2.00870	H	6.39650	6.93351	7.19084
Li	5.01814	2.52186	0.08284	H	3.85612	4.45503	2.01324	H	7.87216	6.37270	3.40236
Li	7.49676	0.07719	10.24065	H	0.57726	3.90731	8.36592	H	6.92501	8.72303	3.19656
Li	7.53183	0.01748	5.23884	H	4.44905	1.18027	8.40532	H	7.08968	6.71007	1.33002
Li	5.02559	2.51608	5.10001	H	3.65529	3.07015	7.12414	H	7.84374	8.44528	1.14977
Li	10.01847	5.02624	10.32571	H	1.36898	1.95744	7.15599	H	6.70716	8.00434	9.06196
Li	2.57641	7.49225	5.24798	H	3.10459	1.50847	3.15274	H	8.27585	7.05658	9.05626
Li	9.57523	7.14726	2.26062	H	1.89862	3.70728	3.17496	H	9.55450	9.27224	6.44813
Li	2.59596	5.00465	7.77728	H	2.04352	1.70419	1.28218	H	5.42585	5.86255	6.50150
Li	10.02154	7.55569	10.27994	H	2.96412	3.31703	1.31523	H	9.07120	5.41468	3.88289
Li	2.54023	4.99264	10.26764	H	1.67601	2.96316	9.04899	H	5.80719	9.58270	3.96893
Li	2.53852	5.02787	5.22721	H	3.32936	2.09517	9.09903	**H**	**2.08925**	**9.46697**	**3.45623**
Li	9.83700	7.25915	5.38479	H	4.59428	4.18367	6.44846				
Li	5.02706	5.02437	0.02667	H	0.52488	0.80712	6.42049				
Li	7.45857	7.55720	5.22372	H	4.27442	0.53983	3.68263				
Li	5.03649	7.52416	2.59592	H	0.79566	4.61881	3.89817				
Li	7.49834	4.98661	7.79138	H	6.16306	0.57588	1.99351				
Li	5.03684	7.53022	0.08773	H	8.86863	4.44080	1.99774				
Li	7.51606	5.02850	10.27982	H	5.57305	3.86667	8.39174				
Li	7.45480	4.97316	5.31171	H	9.45850	1.14836	8.34220				
Li	5.02531	7.51467	5.11340	H	8.65189	3.06028	7.16267				
N	1.12566	1.25351	1.18785	H	6.36721	1.95160	7.12587				
N	3.86351	3.80302	1.21745	H	8.14876	1.28082	3.18007				
N	1.25219	3.89418	9.14192	H	6.98684	3.63969	3.20712				
N	3.77696	1.17494	9.18460	H	7.08232	1.71187	1.33583				
N	3.66840	3.75023	6.35225	H	7.95142	3.35667	1.25501				
N	1.42062	1.30498	6.36334	H	6.69579	2.95089	9.08044				
N	3.71111	1.34901	3.96848	H	8.36173	2.09692	9.02511				
N	1.25461	3.70403	3.97739	H	9.55179	4.19660	6.47840				
N	6.17017	1.25384	1.21946	H	5.45777	0.80891	6.46215				
N	8.87395	3.80366	1.19057	H	9.32477	0.48520	3.92826				
N	6.24465	3.86896	9.17109	H	5.85206	4.57842	3.84290				
N	8.79287	1.17023	9.12596	H	1.29748	5.59271	1.95864				
N	8.64495	3.72691	6.37968	H	3.89480	9.45228	2.00115				
N	6.36513	1.27613	6.34951	H	0.63258	8.89136	8.32360				
N	8.78231	1.35434	3.98691	H	4.48229	6.18374	8.39782				
N	6.30183	3.66475	3.97488	H	3.59633	8.12142	7.20751				
N	1.09952	6.29424	1.23314	H	1.35483	6.87918	7.22186				
N	3.88263	8.79877	1.20766	H	3.15537	6.33699	3.16885				
N	1.25130	8.89511	9.14571	H	1.52609	7.99223	3.05532				
N	3.80074	6.16582	9.16813	H	1.99209	6.79271	1.14178				
N	3.69087	8.76310	6.40996	H	2.97438	8.33359	1.31358				