

## Supplementary Material

Optimized coordinates:

### *cis*-H<sub>2</sub>L

C	5.076561	-1.260452	0.217991
C	5.546898	0.045828	-0.024380
C	4.724410	1.154641	-0.257287
C	3.335485	0.915268	-0.248006
C	2.819017	-0.388524	-0.019509
C	3.697994	-1.456123	0.215920
O	2.445443	1.912859	-0.462552
N	1.426493	-0.430744	-0.043060
C	0.729351	-1.511973	0.002898
C	-0.729345	-1.511996	-0.003483
N	-1.426513	-0.430803	0.042918
C	-2.819031	-0.388555	0.019395
C	-3.335450	0.915251	0.247954
O	-2.445359	1.912787	0.462515
C	-3.698054	-1.456129	-0.215971
C	-5.076615	-1.260415	-0.217973
C	-5.546898	0.045883	0.024393
C	-4.724368	1.154674	0.257267
C	6.023329	-2.447683	0.487034
C	7.508276	-2.039559	0.444954
C	5.728826	-3.035887	1.887553
C	5.798612	-3.541583	-0.583961
C	5.296011	2.563943	-0.511472
C	4.857110	3.062636	-1.910388
C	4.787112	3.541176	0.576859
C	6.836829	2.581031	-0.471402
C	-5.295919	2.563986	0.511508
C	-4.786959	3.541302	-0.576719
C	-6.836734	2.581167	0.471397
C	-4.857008	3.062541	1.910475
C	-6.023434	-2.447628	-0.486918
C	-7.508367	-2.039469	-0.444699
C	-5.729074	-3.035842	-1.887464
C	-5.798646	-3.541528	0.584059
H	6.615366	0.207205	-0.026099
H	3.289214	-2.442572	0.413413
H	1.566735	1.470838	-0.386058
H	1.191217	-2.506188	0.039175
H	-1.191174	-2.506212	-0.040174
H	-3.289325	-2.442608	-0.413416
H	-6.615360	0.207297	0.026149
H	8.136277	-2.915932	0.641036
H	7.795475	-1.641290	-0.534845
H	7.747542	-1.286662	1.204514
H	6.389238	-3.887493	2.092709
H	5.889199	-2.284928	2.669480

H	4.695506	-3.388969	1.972396
H	6.459555	-4.398110	-0.402191
H	4.767565	-3.911145	-0.579409
H	6.010078	-3.155907	-1.587837
H	5.261215	4.066113	-2.093255
H	5.237843	2.398435	-2.695479
H	3.769955	3.110382	-1.997966
H	5.186559	4.546185	0.392593
H	3.697161	3.602536	0.584850
H	5.122332	3.222778	1.571178
H	7.190030	3.601629	-0.656295
H	7.228605	2.270232	0.504151
H	7.278026	1.937231	-1.241305
H	-5.186358	4.546312	-0.392349
H	-3.697008	3.602610	-0.584705
H	-5.122198	3.223030	-1.571073
H	-7.189877	3.601780	0.656318
H	-7.228496	2.270427	-0.504180
H	-7.277999	1.937371	1.241264
H	-5.261137	4.065986	2.093461
H	-5.237695	2.398237	2.695500
H	-3.769849	3.110306	1.998018
H	-8.136408	-2.915829	-0.640710
H	-7.795459	-1.641180	0.535124
H	-7.747691	-1.286575	-1.204245
H	-6.389530	-3.887429	-2.092562
H	-5.889492	-2.284879	-2.669377
H	-4.695771	-3.388953	-1.972395
H	-6.459623	-4.398042	0.402346
H	-4.767609	-3.911116	0.579422
H	-6.010018	-3.155847	1.587953
H	-1.566669	1.470715	0.386009

***trans*-H<sub>2</sub>L**

C	4.868299	1.421520	0.131814
C	5.736611	0.318965	0.007926
C	5.316658	-1.011956	-0.106260
C	3.924808	-1.231924	-0.091289
C	3.014266	-0.148406	0.021705
C	3.500172	1.162271	0.134523
O	3.407599	-2.481098	-0.190552
N	1.678056	-0.552089	0.015903
C	0.675464	0.258811	0.023674
C	-0.675463	-0.258839	0.023687
N	-1.678052	0.552065	0.015888
C	-3.014265	0.148391	0.021709
C	-3.924801	1.231915	-0.091280
O	-3.407580	2.481081	-0.190572
C	-3.500180	-1.162282	0.134524
C	-4.868310	-1.421520	0.131827

C	-5.736616	-0.318961	0.007947
C	-5.316654	1.011958	-0.106246
C	5.378510	2.870634	0.264777
C	6.916320	2.960231	0.232282
C	4.825440	3.723197	-0.901891
C	4.893259	3.466867	1.607564
C	6.314618	-2.179214	-0.245402
C	6.142866	-3.164347	0.937223
C	6.070830	-2.918911	-1.583969
C	7.777967	-1.694255	-0.240617
C	-6.314602	2.179227	-0.245399
C	-6.070793	2.918926	-1.583964
C	-7.777957	1.694289	-0.240631
C	-6.142850	3.164353	0.937229
C	-5.378529	-2.870632	0.264774
C	-6.916341	-2.960212	0.232290
C	-4.825478	-3.723181	-0.901914
C	-4.893274	-3.466891	1.607547
H	6.800131	0.509535	0.002192
H	2.793042	1.980216	0.232951
H	2.433396	-2.342084	-0.145703
H	0.771340	1.350005	0.026547
H	-0.771343	-1.350032	0.026599
H	-2.793058	-1.980237	0.232929
H	-6.800137	-0.509523	0.002214
H	7.224888	4.007590	0.325263
H	7.376429	2.407063	1.058993
H	7.329264	2.577586	-0.708073
H	5.176518	4.759211	-0.819471
H	5.157275	3.327471	-1.868521
H	3.730383	3.744050	-0.908728
H	5.241281	4.501545	1.716500
H	3.800318	3.474982	1.678648
H	5.278024	2.887677	2.454714
H	6.854008	-3.993786	0.837904
H	6.342155	-2.662811	1.891764
H	5.134237	-3.580798	0.972169
H	6.774825	-3.754540	-1.683032
H	5.056279	-3.317526	-1.644960
H	6.228283	-2.243939	-2.433731
H	8.443461	-2.558238	-0.346289
H	7.989922	-1.013471	-1.073238
H	8.043404	-1.188147	0.694909
H	-6.774791	3.754552	-1.683042
H	-5.056243	3.317545	-1.644936
H	-6.228228	2.243950	-2.433725
H	-8.443440	2.558281	-0.346300
H	-7.989913	1.013514	-1.073260
H	-8.043409	1.188176	0.694888
H	-6.853984	3.993799	0.837911
H	-6.342146	2.662815	1.891768
H	-5.134217	3.580795	0.972182

H	-7.224920	-4.007569	0.325258
H	-7.376436	-2.407051	1.059013
H	-7.329288	-2.577548	-0.708055
H	-5.176561	-4.759194	-0.819506
H	-5.157321	-3.327438	-1.868534
H	-3.730421	-3.744040	-0.908764
H	-5.241307	-4.501566	1.716470
H	-3.800332	-3.475022	1.678623
H	-5.278023	-2.887708	2.454709
H	-2.433376	2.342057	-0.145740

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Sn	-0.000010	-0.862370	0.000036
O	2.188166	-1.519835	-0.000109
O	-2.188177	-1.519837	0.000195
N	1.349506	1.005072	0.000085
N	-1.349515	1.005071	0.000067
C	3.100953	-0.596067	-0.000031
C	2.711565	0.793721	0.000057
C	3.675953	1.830552	0.000083
H	3.337858	2.860666	0.000112
C	5.025934	1.541220	0.000074
C	5.400812	0.163026	0.000003
H	6.461365	-0.059839	-0.000014
C	4.514061	-0.900957	-0.000059
C	6.120050	2.622830	0.000081
C	7.004188	2.470872	-1.263098
H	6.407683	2.586027	-2.174845
H	7.492695	1.492563	-1.306988
H	7.791351	3.234234	-1.272926
C	7.004140	2.470952	1.263292
H	6.407604	2.586132	2.175017
H	7.791280	3.234338	1.273118
H	7.492682	1.492665	1.307256
C	5.532576	4.048110	0.000023
H	4.920152	4.238327	0.888500
H	4.920187	4.238270	-0.888489
H	6.344534	4.783385	0.000017
C	4.992432	-2.365969	-0.000152
C	4.471949	-3.090568	-1.267702
H	4.856786	-2.610914	-2.175468
H	3.381762	-3.085242	-1.309588
H	4.812958	-4.133139	-1.269510
C	4.471882	-3.090767	1.267254
H	4.856628	-2.611225	2.175119
H	4.812938	-4.133322	1.268944
H	3.381691	-3.085503	1.309058
C	6.531358	-2.476719	-0.000118
H	6.980973	-2.019597	0.888721
H	6.981020	-2.019527	-0.888897

H	6.816616	-3.534319	-0.000155
C	0.714423	2.156058	0.000141
H	1.239317	3.109584	0.000194
C	-0.714433	2.156057	0.000129
H	-1.239327	3.109583	0.000184
C	-3.100964	-0.596068	0.000100
C	-2.711576	0.793720	0.000048
C	-3.675964	1.830550	-0.000012
H	-3.337871	2.860666	-0.000042
C	-5.025944	1.541217	-0.000037
C	-5.400822	0.163024	-0.000010
H	-6.461373	-0.059841	-0.000066
C	-4.514069	-0.900960	0.000059
C	-6.120047	2.622837	-0.000166
C	-5.532532	4.048101	-0.000612
H	-6.344470	4.783397	-0.000508
H	-4.920390	4.238106	-0.889328
H	-4.919849	4.238428	0.887662
C	-7.004317	2.470602	-1.263214
H	-7.492819	1.492278	-1.306844
H	-6.407913	2.585565	-2.175052
H	-7.791490	3.233954	-1.273126
C	-7.004006	2.471283	1.263183
H	-7.492619	1.493044	1.307406
H	-7.791087	3.234731	1.272938
H	-6.407356	2.586609	2.174814
C	-4.992427	-2.365978	0.000080
C	-6.531351	-2.476763	-0.000012
H	-6.981055	-2.019595	0.888758
H	-6.816583	-3.534369	0.000000
H	-6.980948	-2.019639	-0.888860
C	-4.471974	-3.090630	1.267609
H	-4.856858	-2.611036	2.175387
H	-3.381789	-3.085277	1.309538
H	-4.812957	-4.133209	1.269346
C	-4.471816	-3.090707	-1.267342
H	-3.381624	-3.085424	-1.309098
H	-4.856530	-2.611125	-2.175199
H	-4.812856	-4.133268	-1.269097
C	-0.000209	-1.445992	2.086102
H	0.899720	-1.064991	2.573014
H	-0.002767	-2.537234	2.147613
H	-0.898042	-1.060902	2.573697
C	0.000217	-1.445946	-2.086040
H	0.897975	-1.060700	-2.573651
H	-0.899784	-1.065086	-2.572927
H	0.002961	-2.537186	-2.147567

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Sn	0.000010	0.898131	0.000015
O	-2.264209	1.524973	-0.000141

O	2.264226	1.524974	0.000171
N	-1.353105	-0.956166	-0.000016
N	1.353123	-0.956168	0.000047
C	-3.148098	0.610022	-0.000120
C	-2.703775	-0.796573	-0.000045
C	-3.649750	-1.847544	-0.000003
H	-3.307030	-2.874453	0.000058
C	-5.002448	-1.571010	-0.000001
C	-5.421446	-0.187939	-0.000068
H	-6.487965	-0.003624	-0.000043
C	-4.577889	0.895703	-0.000154
C	-6.076436	-2.664291	0.000079
C	-6.959218	-2.511656	-1.266753
H	-6.364172	-2.619020	-2.179873
H	-7.469162	-1.544804	-1.307981
H	-7.730703	-3.288560	-1.273396
C	-6.959069	-2.511618	1.267011
H	-6.363912	-2.618942	2.180063
H	-7.730545	-3.288530	1.273777
H	-7.469019	-1.544770	1.308265
C	-5.473297	-4.082371	0.000065
H	-4.862988	-4.270868	0.890235
H	-4.863133	-4.270913	-0.890195
H	-6.279218	-4.822213	0.000149
C	-5.083870	2.348335	-0.000180
C	-4.579214	3.081492	-1.270475
H	-4.937348	2.585242	-2.179508
H	-3.489690	3.130563	-1.307642
H	-4.964247	4.106777	-1.278731
C	-4.578945	3.081607	1.269938
H	-4.936824	2.585397	2.179092
H	-4.964038	4.106869	1.278218
H	-3.489413	3.130749	1.306828
C	-6.625038	2.414770	-0.000023
H	-7.062303	1.948390	0.889731
H	-7.062476	1.948793	-0.889900
H	-6.937824	3.463201	0.000240
C	-0.700955	-2.123163	0.000002
H	-1.227826	-3.073311	-0.000011
C	0.700971	-2.123164	0.000024
H	1.227839	-3.073314	0.000030
C	3.148112	0.610020	0.000153
C	2.703793	-0.796575	0.000076
C	3.649772	-1.847542	0.000025
H	3.307058	-2.874453	-0.000046
C	5.002469	-1.571001	0.000021
C	5.421463	-0.187929	0.000070
H	6.487980	-0.003610	0.000009
C	4.577897	0.895709	0.000167
C	6.076458	-2.664282	-0.000113
C	5.473314	-4.082357	-0.000413
H	6.279231	-4.822203	-0.000508

H	4.863127	-4.270706	-0.890698
H	4.863026	-4.271040	0.889731
C	6.959235	-2.511391	-1.266917
H	7.469175	-1.544527	-1.307950
H	6.364185	-2.618571	-2.180055
H	7.730723	-3.288292	-1.273722
C	6.959095	-2.511876	1.266849
H	7.469079	-1.545054	1.308289
H	7.730546	-3.288814	1.273466
H	6.363936	-2.619356	2.179880
C	5.083834	2.348354	0.000168
C	6.625001	2.414877	-0.000152
H	7.062562	1.948894	0.889663
H	6.937727	3.463325	-0.000409
H	7.062199	1.948557	-0.889970
C	4.579262	3.081462	1.270523
H	4.937521	2.585223	2.179512
H	3.489737	3.130459	1.307802
H	4.964228	4.106772	1.278753
C	4.578720	3.081618	-1.269878
H	3.489178	3.130648	-1.306665
H	4.936564	2.585474	-2.179082
H	4.963707	4.106920	-1.278160
C	0.000035	1.563685	2.051300
H	-0.897273	1.201642	2.556089
H	0.001664	2.656091	2.066048
H	0.895884	1.199013	2.556802
C	-0.000028	1.563690	-2.051266
H	-0.895829	1.198928	-2.556788
H	0.897327	1.201738	-2.556036
H	-0.001769	2.656096	-2.066011

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Sn	0.000007	-0.844627	-0.000003
O	2.207849	-1.545704	-0.000085
O	-2.207833	-1.545706	0.000080
N	1.340905	0.964386	-0.000001
N	-1.340890	0.964383	-0.000007
C	3.125284	-0.608675	-0.000018
C	2.715207	0.772700	0.000016
C	3.667550	1.808777	0.000056
H	3.316604	2.835174	0.000078
C	5.036982	1.537148	0.000058
C	5.428446	0.180788	0.000018
H	6.491014	-0.038520	-0.000005
C	4.530225	-0.892365	-0.000002
C	6.109811	2.644043	0.000067
C	7.001727	2.518606	-1.260719
H	6.400640	2.620520	-2.171333
H	7.504060	1.547189	-1.304957
H	7.775933	3.298026	-1.271678

C	7.001596	2.518725	1.260958
H	6.400413	2.620705	2.171500
H	7.775788	3.298159	1.271933
H	7.503945	1.547321	1.305332
C	5.496576	4.059256	-0.000030
H	4.877178	4.234018	0.886608
H	4.877289	4.233944	-0.886760
H	6.294382	4.812334	-0.000012
C	5.017842	-2.355838	-0.000071
C	4.497858	-3.084941	-1.264865
H	4.893372	-2.612117	-2.172437
H	3.407797	-3.055014	-1.306758
H	4.822582	-4.134822	-1.261608
C	4.497968	-3.085044	1.264711
H	4.893601	-2.612324	2.172286
H	4.822652	-4.134938	1.261318
H	3.407914	-3.055078	1.306729
C	6.557143	-2.469184	-0.000139
H	7.005936	-2.008744	0.887925
H	7.005882	-2.008356	-0.888031
H	6.843469	-3.528168	-0.000377
C	0.699355	2.145308	-0.000004
H	1.238826	3.090159	-0.000005
C	-0.699342	2.145307	-0.000009
H	-1.238815	3.090156	-0.000013
C	-3.125271	-0.608679	0.000013
C	-2.715192	0.772695	-0.000023
C	-3.667531	1.808776	-0.000062
H	-3.316582	2.835171	-0.000081
C	-5.036964	1.537151	-0.000061
C	-5.428432	0.180794	-0.000017
H	-6.491001	-0.038515	0.000014
C	-4.530217	-0.892363	0.000001
C	-6.109792	2.644049	-0.000063
C	-5.496557	4.059261	-0.000009
H	-6.294364	4.812339	0.000031
H	-4.877225	4.234025	-0.886693
H	-4.877206	4.233949	0.886676
C	-7.001613	2.518706	-1.260926
H	-7.503956	1.547299	-1.305271
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C	-5.044756	1.778193	-0.001052
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H	-4.777306	2.088363	2.150889
H	-4.829402	3.585999	1.205335
C	0.078103	0.523542	-2.174679
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H	0.931168	0.515747	2.591290
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