Supporting Information: "Exploring N_2 activation using novel Lewis acid/base pairs: computational insight into frustrated Lewis pair reactivity"

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1 Validation of the computational methodology

The theory level used in this work (ωB97XD/6-311++G(2df,2p)//ωB97XD/6-31+G(d)) has been validated by comparison with higher-level theoretical data. We provide a comparison of geometrical parameters, interaction energies, hydrogen affinity values (HIA) and electrophilicity indexes with those reported in the literature.

Regarding the geometrical parameters, we have compared the B-N bond distance and angle in addition to the interaction energy for the reaction LA + N_2 $\rightarrow$ LA-N_2, from Phys. Chem. Chem. Phys. 25, 21006 (2023), where the authors use the following level of theory: M06-2X/jun-cc-pVTZ:

Table 1: Boron-nitrogen bond distance (R_{BN}), in Å, and angle (α), in degrees. Interaction energy (ΔH), in kcal/mol.

	α		$\mathbf{R}_{BN}$		$\mathbf{\Delta H}$	
	jun-cc-pVTZ	This work	jun-cc-pVTZ	This work	jun-cc-pVTZ	This work
LA-8a	102.3	102.7	1.594	1.579	-5.0	-5.2
LA-8f	104.3	103.9	1.622	1.619	-14.7	-12.4

Regarding the geometrical parameters, we have compared the B-P bond distance and interaction energy for the reaction LA + LB $\rightarrow$ LA-LB, from ACS Omega 7, 48493-48505 (2022), where the authors use the following level of theory: M06-2X/def2-TZVP:

Table 2: Boron-phosphorus bond distance (R_{BP}), in Å. Interaction energy (ΔH and ΔG), in kcal/mol.

	$\mathbf{R}_{BP}$		$\mathbf{\Delta H}$		$\mathbf{\Delta G}$	
	def2-TZVP	This work	def2-TZVP	This work	def2-TZVP	This work
LA-5a-LB-2	1.962	1.977	-44.93	-49.81	-30.00	-34.58
LA-5a-LB-3	2.176	2.202	-13.40	-19.22	1.34	-4.31
LA-5b-LB-2	2.422	2.415	-36.81	-42.18	-25.12	-31.99
LA-5b-LB-3	2.507	2.503	-41.59	-47.00	-47.00	-32.88
LA-5e-LB-2	1.983	2.002	-54.73	-56.63	-36.95	-39.74
LA-5e-LB-3	2.152	2.486	-9.80	-2.25	6.45	13.00

The calculated values for the bond distance and angle show excellent agreement between the jun-cc-pVTZ and our level of theory. The interaction energies are also consistent, with minor differences.

The hydrogen affinity values (in kJ/mol) for five LAs were compared using data from ChemPhysChem 22, 935-943 (2021), where a high-level CCSD(T)/CBS method was employed.

Table 3: Hydrogen affinity (HIA), in kJ/mol.

	LA-8a	LA-8b	LA-8c	LA-8d	LA-8ag
CCSD(T)/CBS	305	296	405	437	481
This work	315	302	403	438	480

The hydrogen affinity values computed in this work are in close agreement with those from CCSD(T)/CBS, with discrepancies within acceptable ranges. This suggests that this level of theory provides reliable estimates for HIA.

We have also validated the global (ω) and local (ω_B) electrophilicity indexes using reference values from Angew. Chem. Int. Ed. 59, 12402 (2020), with the M06-2X/6-311G(d) level of theory.

Table 4: Global (ω) and local (ω_B) electrophilicity indexes, in a.u., occupation of the empty $2p$ orbital ($\eta(2p)$) and boron atom charge (Q_B)

	ω		ω_B		$\eta(2p)$		Q_B	
	6-311G(d)	This work	6-311G(d)	This work	6-311G(d)	This work	6-311G(d)	This work
LA-1	0.88	0.85	-0.57	-0.48	—	—	—	—
LA-5a	1.20	0.93	-1.50	-1.25	0.08	0.08	0.92	0.91
LA-8e	0.97	0.95	-0.67	-0.57	0.22	0.21	1.00	0.98
LA-8g	2.79	2.07	-1.23	-1.05	—	—	—	—

The local electrophilicity index (ω_B) demonstrates good consistency, while the global index (ω) shows larger discrepancies. This is expected, as the global index reflects the overall electron-accepting capability of the entire molecule and is a poorer descriptor of the electrophilicity of the boron site.

In conclusion, the comparisons between all parameters demonstrate good overall agreement higher-level calculations available in the literature, validating the reliability of the computational methodology used in this work.

2 Gibbs free energy values

In this section, the corrected (ΔG^{corr}) and non-corrected (ΔG) Gibbs free energy values for the different interactions and transition states are collected.

Table 5: Corrected (ΔG^{corr}) and non-corrected (ΔG) Gibbs free energy values, in kcal/mol, for the interaction between the different Lewis acids and N_2.

	1	2	3a	4	5a	5b	5c	5d	5e	5f	5g	8a	8f
ΔG^{corr}	6.46	-3.02	3.37	-47.79	-6.99	-6.98	-3.64	-11.48	-13.52	-18.17	4.78	-0.89	-10.99
ΔG	12.98	3.42	9.77	-41.71	-0.27	-0.28	3.07	-4.76	-6.74	-11.39	11.58	4.49	-4.29

Table 6: Corrected (ΔG^{corr}) and non-corrected (ΔG) Gibbs free energy values, in kcal/mol, for the LA-N_2-LB interaction.

	LA-4		LA-5a		LA-5b		LA-5d		LA-5e		LA-5f		LA-8f	
	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG
LB-1	-21.97	-7.53	32.33	47.99	—	—	2.22	17.90	13.85	29.71	-14.15	1.71	1.87	26.44
LB-2	-34.05	-19.02	22.50	39.38	—	—	-9.35	7.56	3.11	20.40	-25.93	-8.63	1.15	17.82
LB-3	-43.35	-28.44	13.93	30.55	—	—	-15.37	1.28	-4.02	12.95	-29.91	-12.94	-8.36	8.10
LB-4	-33.29	-18.08	—	—	—	—	-14.76	2.11	-1.39	15.79	-32.99	-15.81	-6.24	10.47
LB-5	-50.52	-35.31	6.11	23.01	16.81	33.73	-25.24	-8.31	-13.06	4.20	-35.65	-18.38	-9.33	7.42
LB-6	-72.71	-57.27	-17.71	-0.33	-12.39	5.04	-54.64	-37.22	-40.97	-23.12	-75.04	-57.19	-42.80	-25.66

Table 7: Corrected (ΔG^{corr}) and non-corrected (ΔG) Gibbs free energy values, in kcal/mol, for the LA-N_2-LB interaction.

	4	5a	5d	5e	5f	8f
$\Delta \mathbf{G}^{corr}$	-97.72	-15.63	27.49	-25.09	12.37	-12.16
$\Delta \mathbf{G}$	-83.57	1.49	44.04	-7.07	31.62	4.59

Table 8: Corrected (ΔG^{corr}) and non-corrected (ΔG) Gibbs free energy values, in kcal/mol, for the LB-N_2-LB interaction.

	1	2	3	4	5	6
$\Delta \mathbf{G}^{corr}$	132.45	53.41	44.17	131.81	29.08	38.57
$\Delta \mathbf{G}$	147.16	70.03	60.31	148.43	45.79	88.12

Table 9: Corrected (ΔG^{corr}) and non-corrected (ΔG) Gibbs free energy values, in kcal/mol, for the LA-LB interaction.

	LA-4		LA-5a		LA-5b		LA-5d		LA-5e		LA-5f		LA-8f	
	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG
LB-1	-106.20	-98.21	-52.21	-43.21	—	—	-71.76	-62.75	-67.93	-58.80	-86.96	-77.83	-70.36	-61.41
LB-2	-97.20	-88.88	-44.77	-34.58	—	—	-61.94	-51.72	-22.20	-11.64	-42.62	-32.05	-51.29	-41.30
LB-3	-108.47	-100.19	-6.97	2.87	—	—	-26.85	-16.90	2.78	13.00	-10.87	-0.64	-40.00	-30.22
LB-4	-114.80	-106.23	-52.54	-42.38	—	—	-74.90	-64.71	-63.78	-53.32	-86.20	-75.74	-66.08	-56.06
LB-5	-101.93	-93.36	-53.41	-43.18	-46.26	-36.04	-70.79	-60.53	-58.21	-47.66	-75.37	-64.82	-60.51	-50.43
LB-6	-143.94	-130.28	-71.51	-60.82	-74.05	-63.35	-100.11	-89.39	-88.89	-77.77	-117.99	-106.86	-81.61	-71.17

Table 10: Corrected (ΔG^{corr}) and non-corrected (ΔG) Gibbs free energy values, in kcal/mol, for selected transition states corresponding to the LB attack to the LA-N_2 complexes.

	LA-4		LA-5a		LA-5d		LA-5e		LA-5f		LA-8f	
	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG	ΔG^{corr}	ΔG
LB-1	28.70	37.04	39.86	48.53	16.93	21.11	30.06	39.14	8.34	10.65	25.87	34.72
LB-2	23.51	32.45	31.82	41.71	8.46	13.88	22.46	32.96	1.58	2.46	18.98	28.94
LB-3	15.59	24.75	23.57	33.19	3.53	8.66	14.82	24.99			10.29	20.02
LB-5	14.56	23.68	22.76	32.67	0.75	6.20	14.21	24.67	1.23	2.14	13.90	23.93

3 Electroaccepting power of the Lewis acids

Figure S1 shows the LUMO molecular orbitals corresponding to the $2p$ boron orbital of **13** and **5e** LAs, where the effect of pyramidalization in the electron delocalization can be observed. The orthogonal arrangement between the triptycene aryl p-orbitals and the boron $2p$ orbital prevents π-conjugation in **5e**, resulting in lower $\eta(2p)$ values. On the contrary, the boron empty orbital of **13** appears mixed with the molecular orbitals of the aryl groups, leading to higher $\eta(2p)$ and therefore hindering the availability of the empty orbital to interact with N_2. This would explain the difference in the interaction patterns between the two acids despite having both high ω_B values.
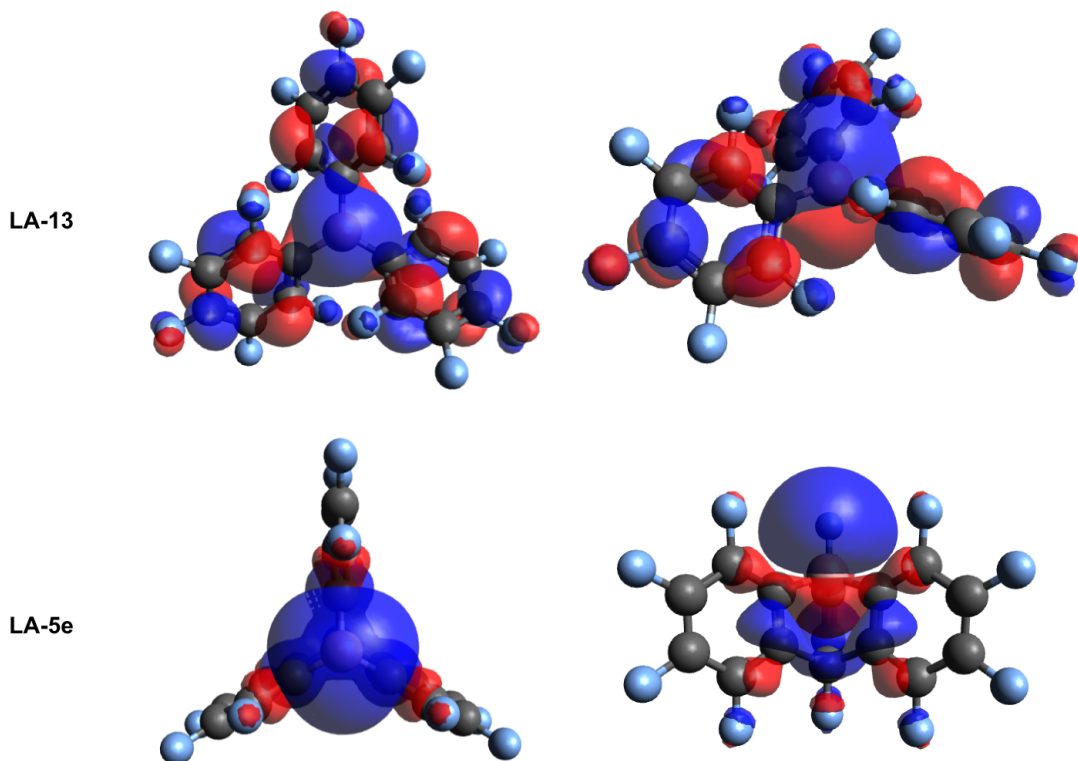
Figure 1: Front and side view of the molecular orbitals of **5e** and **13**, showing the effect of the pyramidalization in the electron delocalization.

4 Principal Component Analysis of the LA-N$_2$ interactions

Figures S2 and S3 presents the front and side views of the molecular orbitals of **2** and the boratriptycene family **5a-g** belonging to the empty boron $2p$ orbital (Al $3p$ and Ga $4p$ orbitals for **5b** and **5c**). The orbital plots were made with Avogadro using the same isovalue (0.03) for optimal comparison between the orbital size. In addition to the parameters identified by the PCA analysis ($\eta(2p)$, α, and ω_B), there also appears to be a connection between the size of the empty $2p$ orbital on boron and the interaction energy with N$_2$ in LAs with a bicyclic structure. The interaction energies increase as the orbital size decreases, with the exception of **5g**, which exhibits the lowest interaction energy despite having the smallest orbital, likely due to the steric hindrance from Cl atoms. We propose that this effect may be linked to Pearson's Hard and Soft Acids and Bases (HSAB) principle, where the hardness of the LA plays a key role. **cita** A smaller orbital suggests a higher hardness (lower polarizability) in line with Pearson's principle, leading to a stronger interaction with a hard base like nitrogen. For instance, comparing **5d** and **5e**, the latter shows a better interaction energy despite having significantly lower electroaccepting power. This can be attributed to the smaller orbital of **5e**, resulting from the electronegative F atoms on the aryl rings, which cause a contraction of the orbital, making it less polarizable and thus harder.
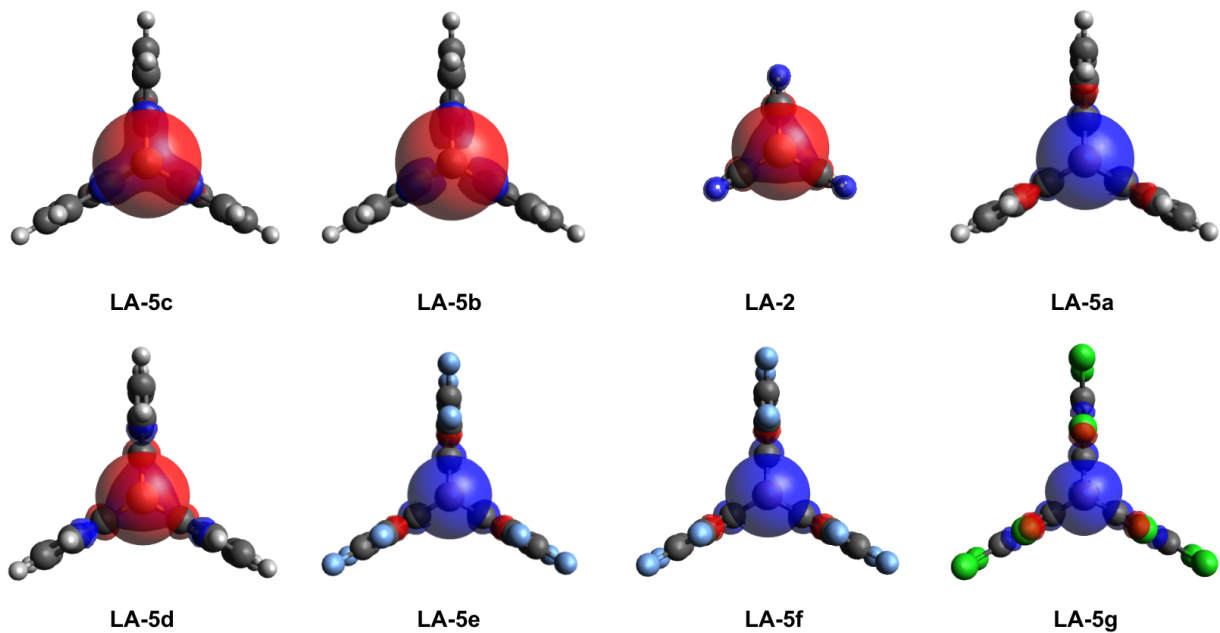
Figure 2: Front view of the molecular orbitals of **5a-g** and **2** LAs showing the empty orbitals of B/Al/Ga.

Figure 3: Side view of the molecular orbitals of **5a-g** and **2** LAs showing the empty orbitals of B/Al/Ga.

5 Nature of the bonding in LA-N$_2$-LB complexes

Table 11: QTAIM analyses for selected LA-N$_2$-LB complexes. Electron density (ρ), its Laplacian ($\nabla^2\rho$), total electron energy density (H), potential electron energy density (G) and kinetic electron energy density (V).
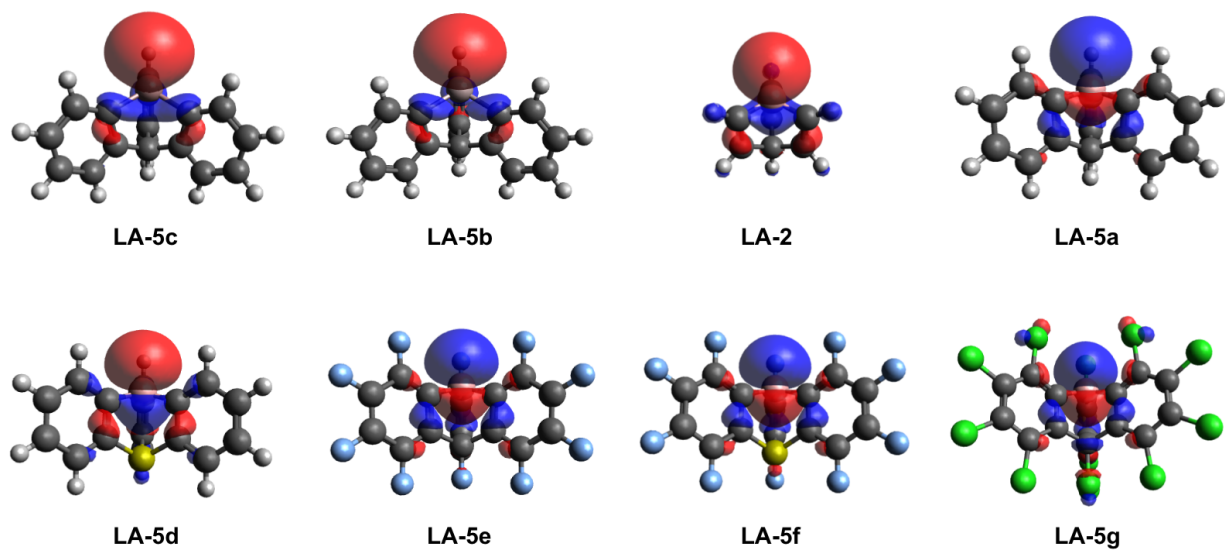
LA	LB	LA-N$_2$					LB-N$_2$				
		ρ_1	$\nabla^2\rho_1$	V$_1$	G$_1$	H$_1$	ρ_2	$\nabla^2\rho_2$	V$_2$	G$_2$	H$_2$
4	1	0.192	0.499	-0.499	0.312	-0.187	0.296	-0.352	-0.389	0.150	-0.238
	2	0.210	0.515	-0.560	0.344	-0.215	0.190	-0.067	-0.387	0.185	-0.202
	3	0.208	0.499	-0.550	0.337	-0.213	0.186	-0.058	-0.376	0.181	-0.195
	4	0.185	0.405	-0.465	0.283	-0.182	0.290	-0.300	-0.369	0.147	-0.222
	5	0.207	0.493	-0.548	0.336	-0.212	0.199	-0.058	-0.421	0.203	-0.218
	6	0.197	0.421	-0.502	0.304	-0.198	0.308	-0.860	-0.451	0.118	-0.333
5a	1	0.142	0.390	-0.335	0.216	-0.119	0.264	-0.214	-0.330	0.139	-0.192
	2	0.154	0.403	-0.371	0.236	-0.135	0.174	-0.269	-0.291	0.112	-0.179
	3	0.157	0.383	-0.376	0.236	-0.140	0.178	-0.189	-0.324	0.139	-0.186
	5	0.159	0.376	-0.382	0.238	-0.144	0.193	-0.155	-0.385	0.173	-0.212
	6	0.162	0.327	-0.381	0.231	-0.149	0.308	-0.853	-0.450	0.118	-0.331
5b	5	0.071	0.318	-0.108	0.094	-0.014	0.186	-0.278	-0.335	0.133	-0.202
	6	0.075	0.334	-0.116	0.100	-0.016	0.305	-0.827	-0.449	0.121	-0.328
5d	1	0.151	0.331	-0.353	0.218	-0.135	0.302	-0.373	-0.395	0.151	-0.244
	2	0.158	0.311	-0.369	0.223	-0.145	0.172	-0.218	-0.301	0.124	-0.177
	3	0.159	0.297	-0.369	0.222	-0.147	0.173	-0.174	-0.311	0.134	-0.177
	4	0.158	0.291	-0.364	0.218	-0.145	0.302	-0.348	-0.394	0.154	-0.241
	5	0.163	0.286	-0.377	0.225	-0.153	0.184	-0.162	-0.357	0.152	-0.199
	6	0.167	0.248	-0.385	0.223	-0.161	0.309	-0.893	-0.476	0.127	-0.350
5e	1	0.157	0.313	-0.366	0.222	-0.144	0.297	-0.354	-0.389	0.150	-0.239
	2	0.160	0.290	-0.370	0.221	-0.149	0.173	-0.241	-0.296	0.118	-0.178
	3	0.159	0.267	-0.364	0.215	-0.149	0.172	-0.197	-0.304	0.127	-0.177
	4	0.159	0.277	-0.365	0.217	-0.148	0.283	-0.268	-0.360	0.147	-0.213
	5	0.164	0.257	-0.377	0.221	-0.156	0.188	-0.165	-0.368	0.163	-0.204
	6	0.171	0.218	-0.390	0.222	-0.168	0.313	-0.909	-0.483	0.128	-0.355
5f	1	0.164	0.263	-0.378	0.222	-0.156	0.317	-0.444	-0.426	0.157	-0.268
	2	0.167	0.211	-0.377	0.215	-0.162	0.171	-0.196	-0.300	0.126	-0.174
	3	0.164	0.193	-0.365	0.207	-0.159	0.168	-0.171	-0.296	0.127	-0.170
	4	0.171	0.213	-0.389	0.221	-0.168	0.322	-0.436	-0.434	0.163	-0.272
	5	0.170	0.180	-0.382	0.213	-0.168	0.175	-0.210	-0.316	0.132	-0.185
	6	0.178	0.149	-0.400	0.219	-0.182	0.315	-0.948	-0.518	0.140	-0.378
8f	1	0.152	0.314	-0.351	0.215	-0.136	0.299	-0.361	-0.393	0.151	-0.242
	2	0.157	0.297	-0.364	0.219	-0.145	0.175	-0.215	-0.309	0.127	-0.181
	3	0.159	0.274	-0.366	0.217	-0.149	0.176	-0.163	-0.324	0.142	-0.182
	4	0.158	0.274	-0.361	0.215	-0.146	0.319	-0.428	-0.430	0.161	-0.268
	5	0.162	0.276	-0.373	0.221	-0.152	0.184	-0.205	-0.347	0.148	-0.199
	6	0.165	0.225	-0.374	0.215	-0.159	0.311	-0.892	-0.471	0.124	-0.347

6 Analysis of the frustration in the LA-LB interaction

Table 12: LA-LB interaction energy (ΔG_{int}), in kcal/mol, and LA-LB bond distances (R), in Å.

LA	LB	ΔG_{int}	R
4	1	-106.20	1.485
	2	-97.20	1.856
	3	-108.47	1.865
	4	-114.80	1.482
	5	-101.93	1.861
	6	-139.00	1.555
5a	1	-52.21	1.569
	2	-44.77	1.978
	3	-14.24	2.202
	5	-53.41	1.965
	6	-71.51	1.636
5b	5	-46.26	2.405
	6	-74.05	2.008
5d	1	-71.76	1.558
	2	-61.94	1.998
	3	-26.85	2.206
	4	-74.90	1.578
	5	-70.79	1.998
	6	-100.11	1.631
5e	1	-67.93	1.547
	2	-50.31	2.002
	3	2.78	2.486
	4	-63.78	1.564
	5	-58.21	2.009
	6	-88.89	1.622
5f	1	-86.96	1.534
	2	-67.15	2.013
	3	-10.87	2.456
	4	-86.20	1.534
	5	-75.37	2.031
	6	-117.99	1.615
8f	1	-70.36	1.559
	2	-51.29	2.034
	3	-40.00	2.154
	4	-66.08	1.580
	5	-60.51	2.034
	6	-81.61	1.652

Table 13: Boron-phosphorous bond distances (R(B-P)), in Å, and LA-LB interaction energies (ΔH and ΔG), in kcal/mol, for selected Lewis acids and bases in comparison with the values from *ACS Omega* **7**, 48493-48505 (2022).

	R(B-P)		ΔH		ΔG	
	Ref.	this work	Ref.	this work	Ref.	this work
5a-2	1.962	1.977	-44.93	-49.81	-30.00	-34.58
5a-3	2.176	2.202	-13.40	-19.22	1.34	-4.31
5b-2	2.422	2.415	-36.81	-42.18	-25.12	-31.99
5b-3	2.507	2.503	-41.59	-47.00	-27.44	-32.88
5e-2	1.983	2.002	-54.73	-56.63	-36.95	-39.74
5e-3	2.152	2.486	-9.80	-2.25	6.45	13.00

7 Cartesian coordinates for all compounds

N₂
```
     2
xyz
  N      0.000000      0.000000     -0.000608
  N      0.000000      0.000000      1.100608
```

LA–1
```
    25
xyz
  B     -0.000477      0.000340      1.413085
  C      1.255148      0.897971      1.114833
  C      1.193447      0.853513     -0.456241
  C      1.322558     -0.600697     -0.947135
  C      0.142748     -1.460378     -0.455860
  C      0.149466     -1.535884      1.115199
  C     -1.180931     -0.845312     -0.947525
  C     -1.335689      0.606493     -0.456796
  C     -0.140882      1.445259     -0.947954
  C     -1.405493      0.638764      1.114248
  H      2.218053      0.490616      1.445837
  H      1.181297      1.940958      1.445553
  H      2.023207      1.446754     -0.861173
  H      1.352877     -0.614679     -2.045245
  H      2.269388     -1.030655     -0.595195
  H      0.241974     -2.475635     -0.860596
  H      1.089564     -1.993103      1.446601
  H     -0.684862     -2.166213      1.445744
  H     -2.026853     -1.450112     -0.595603
  H     -1.207852     -0.865009     -2.045632
  H     -2.264325      1.028093     -0.862151
  H     -0.242045      2.480318     -0.596324
  H     -0.143869      1.478171     -2.046072
  H     -1.534082      1.676563      1.444563
  H     -2.271902      0.053508      1.445129
```

LA–2 bora barrelene
```
    15
xyz
  C      0.000103     -0.000090      1.155394
  H      0.000244     -0.000120      2.246089
  B     -0.000084      0.000112     -1.173946
  C     -1.348354     -0.497452      0.578669
  H     -2.140170     -0.789803      1.263292
  C     -1.426637     -0.525875     -0.756724
  H     -2.298714     -0.847405     -1.313611
  C      0.257757      1.498477     -0.756772
  H      0.415137      2.414502     -1.313705
  C      0.243492      1.416394      0.578601
  H      0.386344      2.248269      1.263223
  C      1.168698     -0.972402     -0.756990
  H      1.883103     -1.566716     -1.314183
  C      1.105061     -0.919111      0.578405
  H      1.754205     -1.458840      1.262836
```

LA–3a
```
   15
xyz
  C       1.076358      0.852510     -0.514808
  C      -0.186056      1.264208      0.340143
  C       0.000255     -0.000520      1.230823
  C       1.188049     -0.471236      0.339166
  C       0.199573     -1.358481     -0.515380
  B       0.000315      0.000600     -1.308110
  C      -1.002107     -0.793152      0.339441
  C      -1.276466      0.506431     -0.514878
  H       0.355500     -2.419649     -0.680188
  H      -0.336339      2.286124      0.690526
  H       2.148487     -0.852039      0.688763
  H      -1.812073     -1.434319      0.689506
  H       0.000563     -0.000931      2.319678
  H      -2.273512      0.901964     -0.679160
  H       1.917233      1.518386     -0.679287
```

LA–3b
```
   12
xyz
  N       1.167482     -0.667027     -0.523844
  C       0.005633     -1.228137      0.296634
  N      -1.161667     -0.677237     -0.522858
  C      -1.066166      0.609626      0.297015
  C      -0.000178     -0.000344      1.233255
  C       1.060979      0.618483      0.297365
  N      -0.005487      1.344900     -0.522917
  B      -0.000715      0.000192     -1.134758
  H       0.010133     -2.287799      0.541791
  H      -1.985919      1.135705      0.542507
  H       1.976358      1.151835      0.543605
  H      -0.000568     -0.000831      2.317932
```

LA–4
```
    4
xyz
  N      -0.858563     -0.312142      0.206443
  B      -0.000182     -0.000303     -0.859174
  N       0.699515     -0.587552      0.206530
  N       0.159204      0.899909      0.206250
```

LA–5a
```
   33
xyz
  C       1.275310     -0.811095     -0.816657
  C       1.204600     -0.766164      0.595487
  C       2.178005     -1.385304      1.365717
  H       2.119906     -1.348246      2.451284
  C       3.232137     -2.055694      0.738922
  H       3.995812     -2.541265      1.339836
  C       3.304805     -2.101954     -0.649686
  H       4.126086     -2.624305     -1.132403
```

```
C    2.325565   -1.479187   -1.429970
H    2.393890   -1.522657   -2.513838
C    0.064944    1.509795   -0.816802
C    0.061427    1.426147    0.595353
C    0.110722    2.578692    1.365615
H    0.107757    2.509851    2.451184
C    0.163978    3.826742    0.738778
H    0.202645    4.730921    1.339679
C    0.167555    3.912810   -0.649829
H    0.208969    4.885268   -1.132508
C    0.118039    2.753376   -1.430159
H    0.121331    2.834292   -2.514023
C   -1.339782   -0.698861   -0.816774
C   -1.265633   -0.659982    0.595353
C    0.000099    0.000034    1.159879
C   -2.288615   -1.193300    1.365531
H   -2.227606   -1.161394    2.451101
C   -3.396270   -1.770831    0.738643
H   -4.198814   -2.189173    1.339495
C   -3.472599   -1.810726   -0.649965
H   -4.335682   -2.260607   -1.132736
C   -2.443472   -1.274308   -1.430199
H   -2.515223   -1.311707   -2.514074
H    0.000031    0.000074    2.253173
B    0.000195   -0.000080   -1.234111
```

LA–5b
```
   33
xyz
C    1.518048   -0.965356   -1.040935
C    1.247300   -0.793174    0.338742
C    2.105593   -1.339028    1.292589
H    1.895525   -1.205404    2.351934
C    3.232807   -2.056017    0.894989
H    3.896433   -2.478141    1.644728
C    3.506829   -2.230319   -0.458961
H    4.385737   -2.789359   -0.768881
C    2.650540   -1.685648   -1.416717
H    2.879422   -1.831251   -2.470087
C    0.077285    1.797021   -1.040820
C    0.063418    1.476615    0.338862
C    0.106801    2.492943    1.292598
H    0.095979    2.244359    2.351980
C    0.163919    3.827578    0.894841
H    0.197316    4.613496    1.644475
C    0.177967    4.151881   -0.459138
H    0.222592    5.192530   -0.769186
C    0.134689    3.137869   -1.416835
H    0.146420    3.408758   -2.470237
C   -1.594847   -0.831796   -1.041057
C   -1.310420   -0.683602    0.338683
C    0.000083   -0.000105    0.795236
C   -2.212387   -1.153860    1.292460
H   -1.991659   -1.038755    2.351819
```

```
  C    −3.397031   −1.771264    0.894803
  H    −4.094611   −2.134700    1.644488
  C    −3.684929   −1.921309   −0.459158
  H    −4.608649   −2.402698   −0.769110
  C    −2.784948   −1.452255   −1.416924
  H    −3.025533   −1.577600   −2.470288
  H     0.000132   −0.000196    1.888372
 Al     0.000289   −0.000049   −1.761968
```

LA−5c
```
   33
xyz
  C     1.512453   −0.961946   −1.024304
  C     1.247750   −0.793525    0.351758
  C     2.111031   −1.342507    1.297713
  H     1.908180   −1.213447    2.358822
  C     3.235481   −2.057647    0.889098
  H     3.904329   −2.482898    1.632263
  C     3.499398   −2.225588   −0.467661
  H     4.376235   −2.783310   −0.785202
  C     2.636688   −1.677007   −1.416990
  H     2.854978   −1.815966   −2.472623
  C     0.076948    1.790662   −1.024293
  C     0.063416    1.477253    0.351763
  C     0.107204    2.499378    1.297688
  H     0.096804    2.259247    2.358800
  C     0.164217    3.830720    0.888947
  H     0.198027    4.622635    1.632094
  C     0.177661    4.143245   −0.467799
  H     0.222178    5.181478   −0.785313
  C     0.134066    3.121789   −1.417104
  H     0.145181    3.380224   −2.472760
  C    −1.589137   −0.828848   −1.024436
  C    −1.311044   −0.683742    0.351626
  C     0.000007   −0.000055    0.794343
  C    −2.218212   −1.156726    1.297518
  H    −2.005071   −1.045516    2.358624
  C    −3.399837   −1.772741    0.888855
  H    −4.102746   −2.139010    1.632000
  C    −3.677155   −1.917448   −0.467906
  H    −4.598590   −2.397887   −0.785480
  C    −2.770516   −1.444898   −1.417200
  H    −2.999896   −1.564619   −2.472839
  H    −0.000029   −0.000086    1.887848
 Ga     0.000116   −0.000052   −1.746553
```

LA−5d
```
   32
xyz
  C    −0.931445   −2.560758    1.539350
  C    −0.521104   −1.432104    0.838572
  C    −0.544695   −1.496540   −0.564317
  C    −0.951117   −2.613828   −1.278934
  C    −1.357015   −3.730626   −0.548721
```

```
C     −1.345605    −3.699737     0.843808
B     −0.000151     0.000202     1.213591
C      1.500610     0.264961     0.838619
C      1.568120     0.276824    −0.564206
C      2.739005     0.483399    −1.278730
C      3.909232     0.689666    −0.548476
C      3.876833     0.683789     0.844048
C      2.683258     0.473365     1.539448
S     −0.000173    −0.000033    −1.430115
C     −1.023983     1.219875    −0.564418
C     −0.980001     1.167390     0.838410
C     −1.752177     2.087204     1.539084
C     −2.531190     3.015557     0.843568
C     −2.552063     3.040882    −0.548961
C     −1.788092     2.130649    −1.279105
H     −1.794886     2.139118    −2.364848
H     −3.162638     3.768856    −1.072430
H     −3.130073     3.729171     1.400477
H     −1.753367     2.088425     2.624465
H      2.749834     0.485407    −2.364468
H      4.844964     0.854733    −1.071859
H      4.794256     0.845461     1.401058
H      2.684799     0.473543     2.624831
H     −0.954833    −2.624100    −2.364682
H     −1.681658    −4.623616    −1.072177
H     −1.663798    −4.575334     1.400751
H     −0.931791    −2.562397     2.624728
```

LA−5e
```
   33
xyz
C      1.481610     2.277525     1.512300
C      0.819062     1.259124     0.873259
C      0.783347     1.204422    −0.537776
C      1.423692     2.189611    −1.269943
C      2.095177     3.221886    −0.607543
C      2.127537     3.270949     0.777578
B      0.000048     0.000013     1.310103
C     −1.499768     0.079725     0.873108
C     −1.434423     0.076189    −0.537897
C     −2.607706     0.138417    −1.270129
C     −3.837470     0.203720    −0.607845
C     −3.896283     0.206940     0.777285
C     −2.713031     0.144221     1.512112
C      0.000155     0.000022    −1.108214
C      0.651481    −1.280470    −0.537847
C      0.681105    −1.338735     0.873174
C      1.231810    −2.421758     1.512151
C      1.768733    −3.478036     0.777334
C      1.741823    −3.425666    −0.607815
C      1.183671    −2.327925    −1.270124
F      1.193083    −2.347648    −2.601005
F      2.251900    −4.429600    −1.314120
F      2.302424    −4.527834     1.391965
```

```
F    1.262917   −2.482781    2.849488
F   −2.629694    0.139420   −2.600993
F   −4.961933    0.263427   −1.314192
F   −5.072292    0.269456    1.391930
F   −2.781375    0.148046    2.849458
F    1.435206    2.208493   −2.600816
F    2.708864    4.166113   −1.313755
F    2.769635    4.258142    1.392280
F    1.519077    2.334742    2.849642
F    0.000325   −0.000060   −2.466488

LA−5f
    32
xyz
 C   −1.782695    2.123430   −1.270400
 C   −1.012120    1.205611   −0.574312
 C   −0.976249    1.163234    0.830816
 C   −1.739454    2.072694    1.525909
 C   −2.527238    3.010983    0.846353
 C   −2.549572    3.037146   −0.545514
 S    0.000101   −0.000074   −1.448817
 C    1.550453    0.273582   −0.574299
 C    1.495792    0.263828    0.830810
 C    2.664875    0.470182    1.526125
 C    3.871417    0.683289    0.846823
 C    3.905425    0.689444   −0.545029
 C    2.730784    0.482045   −1.270104
 B    0.000254   −0.000174    1.231143
 C   −0.519110   −1.427389    0.830720
 C   −0.925423   −2.542931    1.525882
 C   −1.344594   −3.694164    0.846431
 C   −1.356233   −3.726570   −0.545438
 C   −0.948107   −2.605694   −1.270379
 C   −0.538097   −1.479548   −0.574403
 F   −1.801074    2.145120   −2.593328
 F   −3.292508    3.921981   −1.178945
 F   −3.251536    3.873873    1.523216
 F   −1.741080    2.074964    2.853712
 F    2.759087    0.487213   −2.593027
 F    5.043254    0.890591   −1.178271
 F    4.980703    0.879298    1.523872
 F    2.667425    0.470537    2.853927
 F   −0.957723   −2.632584   −2.593302
 F   −1.751307   −4.812318   −1.178836
 F   −1.730013   −4.752739    1.523344
 F   −0.926380   −2.545457    2.853683

LA−5g
    33
xyz
 C    1.243293   −2.444271   −1.320611
 C    0.672013   −1.321318   −0.692686
 C    0.673040   −1.323745    0.714071
 C    1.188897   −2.338554    1.483462
```

```
C     1.755134    −3.451965     0.866536
C     1.776655    −3.493602    −0.531098
C     0.000187    −0.000218    −1.285605
Cl    0.000583    −0.001195    −3.049252
B     0.000183    −0.000355     1.133814
C    −1.482302     0.078470     0.713856
C    −1.479807     0.078722    −0.692886
C    −2.737880     0.146613    −1.320754
C    −3.913353     0.208816    −0.531336
C    −3.866472     0.205426     0.866347
C    −2.619084     0.138714     1.483268
Cl   −3.000988     0.162700    −3.035241
Cl   −5.465698     0.292189    −1.290200
Cl   −5.301526     0.281393     1.816956
Cl   −2.440872     0.128429     3.210604
Cl    1.107882    −2.179745     3.210870
Cl    2.406222    −4.733053     1.817167
Cl    2.481639    −4.879222    −1.289940
Cl    1.363634    −2.679376    −3.034922
C     0.809857     1.244036     0.713888
C     1.430822     2.198219     1.483248
C     2.111178     3.245851     0.866306
C     2.135587     3.286037    −0.531369
C     1.493759     2.299271    −1.320736
C     0.808007     1.242327    −0.692864
Cl    1.335001     2.048004     3.210615
Cl    1.635708     2.521461    −3.035221
Cl    2.981542     4.590287    −1.290355
Cl    2.895147     4.450191     1.816976
```

LA−6
```
   36
xyz
 O    −0.507585    −1.272336    −1.692560
 O     1.355587     0.196622    −1.692716
 O    −0.848164     1.075744    −1.692663
 C    −1.421253    −1.472569    −0.685647
 C    −1.214679    −0.876860     0.568088
 C    −2.172285    −1.122441     1.556231
 C    −3.275006    −1.938035     1.322245
 C    −3.438532    −2.535114     0.074190
 C    −2.510381    −2.299255    −0.933417
 C     1.986006    −0.494459    −0.685854
 C     1.366881    −0.613335     0.567927
 C     2.058254    −1.319939     1.556053
 C     3.315883    −1.867190     1.322109
 C     3.914756    −1.710299     0.074059
 C     3.246526    −1.024401    −0.933607
 C    −0.564800     1.967133    −0.685747
 C    −0.152195     1.490484     0.568000
 C     0.114007     2.442676     1.556039
 C    −0.040825     3.805443     1.321984
 C    −0.476135     4.245519     0.073916
 C    −0.736130     3.323695    −0.933562
```

```
C       0.000082      0.000094      0.921982
B      -0.000084      0.000005     -1.750566
H      -2.045069     -0.665006      2.535000
H      -3.997671     -2.111889      2.113596
H      -4.290627     -3.180121     -0.118670
H      -2.615535     -2.740448     -1.919311
H       1.598442     -1.438533      2.534792
H       3.827696     -2.406161      2.113477
H       4.899398     -2.125816     -0.118694
H       0.446677      2.103851      2.534791
H      -1.065690      3.635337     -1.919437
H       0.000190      0.000130      2.014964
H       3.681267     -0.894933     -1.919485
H       0.170087      4.518250      2.113288
H      -0.608661      5.305953     -0.118968
```

LA–7
```
    58
xyz
C      -1.735048      3.054862     -0.040863
H      -1.827105      4.125110      0.083520
C      -0.499418      2.340027     -0.204668
C      -2.782284      2.146381     -0.040815
C       0.900087      2.604218     -0.138825
N      -0.901895      1.036231     -0.354758
C      -2.250834      0.824048     -0.220300
H      -3.827989      2.385227      0.097482
C       1.397328      3.981644      0.069824
C       1.830848      1.525238     -0.202127
C      -2.722714     -0.521104     -0.181644
C       2.403226      4.495310     -0.758329
C       0.879607      4.780825      1.096898
C       3.227491      1.318483      0.058561
N       1.346359      0.254748     -0.397123
C      -1.790267     -1.599506     -0.216803
C      -4.172143     -0.786267     -0.055330
C       2.877099      5.789234     -0.565908
H       2.795348      3.888697     -1.570531
C       1.359080      6.072670      1.288331
H       0.124235      4.379316      1.767146
H       3.945163      2.100628      0.265831
C       3.487157     -0.043383      0.056212
C       2.264141     -0.748817     -0.204354
N      -0.455917     -1.293385     -0.303237
C      -1.798122     -3.033788     -0.130850
C      -5.077981     -0.162453     -0.922531
C      -4.654658     -1.655259      0.931426
H       3.649325      6.182591     -1.219757
C       2.356086      6.579661      0.456713
H       0.959641      6.681237      2.093730
H       4.442487     -0.507066      0.261410
C       1.797257     -2.096186     -0.157085
C       0.397756     -2.363314     -0.210878
C      -0.488957     -3.490756     -0.126227
```
```
                              15
```

```
H    −2.683326    −3.652499    −0.075459
H    −4.709924     0.494986    −1.705928
C    −6.442324    −0.409253    −0.807208
H    −3.963028    −2.118077     1.630373
C    −6.020037    −1.896392     1.045663
H     2.727679     7.588560     0.606726
C     2.768169    −3.198925     0.007193
H    −0.181607    −4.525852    −0.066762
H    −7.135869     0.070187    −1.491074
C    −6.915410    −1.275879     0.176301
H    −6.386038    −2.563271     1.820215
C     3.891379    −3.271888    −0.826607
C     2.583229    −4.174583     0.995119
H    −7.980335    −1.466589     0.265958
H     4.030277    −2.531920    −1.610492
C     4.809528    −4.306331    −0.677772
C     3.505740    −5.205312     1.142986
H     1.733800    −4.108033     1.669707
H     5.671219    −4.360427    −1.335883
C     4.618459    −5.274238     0.306450
H     3.360079    −5.950951     1.918481
H     5.336276    −6.080288     0.422603
B    −0.004192    −0.001707    −0.419360
```

LA−8a
```
     4
xyz
 B     0.112277     0.000000    −0.039695
 H    −0.106115     0.000000     1.136525
 H     1.240380    −0.000000    −0.438536
 H    −0.796880     0.000000    −0.817270
```

LA−8b
```
     4
xyz
 B    −0.000004     0.000000     0.000000
 F     0.658936     1.142338     0.000000
 F     0.659828    −1.141830    −0.000000
 F    −1.318760    −0.000505     0.000000
```

LA−8c
```
     4
xyz
 B     0.000000     0.000011     0.000000
Cl     0.899363     1.499216     0.000000
Cl     0.848741    −1.528393     0.000000
Cl    −1.748104     0.029173    −0.000000
```

LA−8d
```
     4
xyz
 B    −0.000015     0.000017    −0.000000
Br     1.267033    −1.408195    −0.000000
Br    −1.853081    −0.393175    −0.000000
```

```
Br      0.586063      1.801391      0.000000
```

LA–8e
```
    13
xyz
  B      0.072028      0.000000     -0.039226
  C     -0.169879      0.000000      1.524346
  C      1.565082     -0.000000     -0.569523
  C     -1.117118      0.000000     -1.077414
  H      1.662719     -0.000000     -1.661110
  H      2.108504      0.873449     -0.180372
  H      2.108504     -0.873449     -0.180372
  H     -2.121793      0.000000     -0.641835
  H     -1.028439      0.871837     -1.743168
  H     -1.028439     -0.871837     -1.743168
  H     -1.222580      0.000000      1.826470
  H      0.316795     -0.872816      1.984212
  H      0.316795      0.872816      1.984212
```

LA–8f
```
    13
xyz
  B     -0.052726     -0.007189     -0.000000
  C      1.565218     -0.012102     -0.000000
  C     -0.808097      1.422106     -0.000000
  C     -0.819393     -1.425067     -0.000000
  F     -2.146007      1.347331     -0.000000
  F     -0.447388      2.126226      1.091946
  F     -0.447388      2.126226     -1.091946
  F     -2.155930     -1.363443     -0.000000
  F     -0.449995     -2.123108     -1.094853
  F     -0.449995     -2.123108      1.094853
  F      2.111264     -1.237366     -0.000000
  F      2.025873      0.630883     -1.091555
  F      2.025873      0.630883      1.091555
```

LA–8g
```
    34
xyz
  B     -0.000000     -0.000000     -0.000559
  C      0.390041      1.300134     -0.783871
  C      1.092563      3.642918     -2.194760
  C      1.183781      1.264094     -1.933153
  C     -0.034662      2.567186     -0.376022
  C      0.291118      3.727490     -1.061966
  C      1.548006      2.404636     -2.632765
  C     -0.000000     -0.000000      1.566675
  C     -0.000000     -0.000000      4.390278
  C      0.997058      0.638511      2.308451
  C     -0.997058     -0.638511      2.308451
  C     -1.019723     -0.639894      3.694979
  C      1.019723      0.639894      3.694979
  C     -0.390041     -1.300134     -0.783871
  C     -1.092563     -3.642918     -2.194760
```

```
C      −1.183781     −1.264094     −1.933153
C       0.034662     −2.567186     −0.376022
C      −0.291118     −3.727490     −1.061966
C      −1.548006     −2.404636     −2.632765
F      −0.150578      4.912412     −0.648871
F      −0.816117      2.696765      0.702423
F       1.422326      4.742588     −2.856977
F       2.321568      2.326325     −3.712250
F       1.653704      0.096093     −2.386345
F      −1.653704     −0.096093     −2.386345
F       0.816117     −2.696765      0.702423
F       0.150578     −4.912412     −0.648871
F      −2.321568     −2.326325     −3.712250
F      −1.422326     −4.742588     −2.856977
F      −1.999131     −1.244781      4.361826
F      −0.000000     −0.000000      5.715620
F       2.004081      1.258769      1.682570
F       1.999131      1.244781      4.361826
F      −2.004081     −1.258769      1.682570
```

LB−1
```
    9
xyz
 N     −2.761101     −0.150035      0.184479
 H     −3.623586      0.378589      0.154827
 H     −2.692660     −0.734437      1.008147
 N     −0.453723     −0.008429      0.176313
 H      0.372508      0.481381     −0.137594
 H     −0.450808     −0.982236     −0.099983
 N     −1.817941      1.875568     −0.420839
 H     −0.933272      2.314246     −0.668449
 C     −1.656965      0.661212     −0.050441
```

LB−2
```
   34
xyz
 P      0.000000     −0.000000      1.261388
 C      0.376410      1.606362      0.438904
 C     −0.191830      2.756669      1.001316
 C      1.183798      1.741511     −0.695229
 C      0.021900      4.009073      0.432245
 H     −0.809612      2.670173      1.892698
 C      1.409397      2.996858     −1.258197
 H      1.640462      0.863611     −1.143822
 C      0.826210      4.131988     −0.699788
 H     −0.431363      4.889907      0.878450
 H      2.041178      3.085525     −2.137828
 H      1.001973      5.109189     −1.140843
 C      1.202945     −1.129161      0.438904
 C      0.916294     −1.895954     −0.695229
 C      2.483261     −1.212205      1.001316
 C      1.890656     −2.719003     −1.258197
 H     −0.072322     −1.852487     −1.143822
 C      3.461009     −2.023502      0.432245
```

```
H       2.717244    -0.633942    1.892698
C       3.165302    -2.781513   -0.699788
H       1.651554    -3.310474   -2.137828
H       4.450466    -2.071382    0.878450
H       3.923701    -3.422328   -1.140843
C      -1.579355    -0.477201    0.438904
C      -2.291431    -1.544464    1.001316
C      -2.100091     0.154443   -0.695229
C      -3.482909    -1.985571    0.432245
H      -1.907632    -2.036231    1.892698
C      -3.300054    -0.277855   -1.258197
H      -1.568140     0.988876   -1.143822
C      -3.991511    -1.350475   -0.699788
H      -4.019102    -2.818525    0.878450
H      -3.692732     0.224949   -2.137828
H      -4.925674    -1.686860   -1.140843
```

LB−3
```
   40
xyz
 P     -0.000000     0.000000    0.711900
 C      0.006422     1.790194    0.006391
 C      1.547142    -0.900658    0.006391
 C     -1.553564    -0.889535    0.006391
 C      1.396727     2.418304    0.222602
 H      2.157534     2.013640   -0.448199
 H      1.331235     3.495073    0.018569
 H      1.740663     2.301160    1.256114
 C     -0.950173     2.627293    0.884675
 H     -0.866219     3.684704    0.599166
 H     -1.998185     2.348212    0.775170
 H     -0.687352     2.542480    1.944647
 C     -0.375443     1.975497   -1.470553
 H     -0.269695     3.035040   -1.742798
 H      0.265032     1.397906   -2.142143
 H     -1.412891     1.697024   -1.671592
 C      2.750389    -0.490772    0.884675
 H      3.624157    -1.092185    0.599166
 H      3.032704     0.556373    0.775170
 H      2.545528    -0.675976    1.944647
 C      1.395950    -2.418753    0.222602
 H      0.665097    -2.875299   -0.448199
 H      2.361204    -2.900420    0.018569
 H      1.122532    -2.658038    1.256114
 C      1.898552    -0.662605   -1.470553
 H      2.176111     0.375087   -1.671592
 H      2.763269    -1.283957   -1.742798
 H      1.078106    -0.928477   -2.142143
 C     -1.523109    -1.312891   -1.470553
 H     -2.493575    -1.751083   -1.742798
 H     -1.343138    -0.469428   -2.142143
 H     -0.763221    -2.072111   -1.671592
 C     -1.800216    -2.136521    0.884675
 H     -2.757938    -2.592520    0.599166
```

```
H    -1.034519    -2.904585     0.775170
H    -1.858176    -1.866504     1.944647
C    -2.792676     0.000449     0.222602
H    -2.863195     0.356878     1.256114
H    -2.822631     0.861659    -0.448199
H    -3.692440    -0.594653     0.018569
```

LB-4
```
   33
xyz
 P    -2.357717     1.488014     0.236952
 N    -3.653219     0.991931    -0.748996
 N    -1.216845     0.307926    -0.189216
 N    -1.985448     2.993413    -0.411655
 C    -4.159728    -0.361581    -0.535848
 H    -4.875906    -0.403269     0.299170
 H    -3.341200    -1.050889    -0.319176
 H    -4.672046    -0.704120    -1.443470
 C    -4.741698     1.946064    -0.934661
 H    -4.340807     2.940903    -1.133930
 H    -5.395472     2.005021    -0.050404
 H    -5.347060     1.629400    -1.792300
 C    -1.027315    -0.218724    -1.530360
 H    -1.931895    -0.086283    -2.125398
 H    -0.799163    -1.292192    -1.477204
 H    -0.191920     0.278466    -2.047961
 C    -0.021289     0.203498     0.634223
 H    -0.212375     0.615640     1.626527
 H     0.825868     0.748102     0.186748
 H     0.267922    -0.850412     0.737792
 C    -1.450249     4.039311     0.447118
 H    -1.854382     3.921197     1.452224
 H    -1.744486     5.017089     0.045078
 H    -0.350157     4.003211     0.499156
 C    -1.515569     3.059025    -1.784230
 H    -2.049827     2.337073    -2.407245
 H    -0.433444     2.864778    -1.867349
 H    -1.711680     4.061111    -2.184262
 N    -2.515484     1.676321     1.772017
 C    -2.886258     0.612054     2.680380
 H    -3.960485     0.370426     2.638624
 H    -2.673944     0.926398     3.709485
 H    -2.338772    -0.332552     2.513064
```

LB-5
```
   35
xyz
 P    10.383507    12.680786     4.124096
 N     7.049282    11.829063     4.289549
 N     9.752724    12.407760     5.698120
 N     9.279292    13.830699     3.484828
 N     9.930563    11.244698     3.297898
 C     7.332947    11.628851     5.691934
 H     6.750344    10.769659     6.067318
```

```
H      6.972934    12.508774     6.239013
C      8.806058    11.363626     6.040395
H      8.881072    11.179261     7.121314
H      9.108644    10.431693     5.547941
C      7.428177    10.800387     3.348525
H      6.611161    10.645161     2.622626
H      7.533566     9.858587     3.900874
C      8.705346    11.077478     2.539904
H      8.855567    10.251044     1.831099
H      8.534846    11.975110     1.933457
C      6.844265    13.174673     3.805309
H      5.937944    13.600147     4.270192
H      6.642328    13.119647     2.728568
C      7.994112    14.158980     4.071520
H      7.696723    15.150728     3.702775
H      8.111848    14.257529     5.157375
C     10.157353    13.311810     6.754268
H     10.993458    13.929029     6.406000
C     10.811653    10.100252     3.399929
H     11.764707    10.411689     3.842664
C      9.633235    14.490331     2.245404
H     10.684411    14.286933     2.010938
H     10.400532     9.296646     4.032092
H     11.023385     9.676039     2.408151
H     10.494799    12.756355     7.640824
H      9.350963    13.994292     7.067960
H      9.511394    15.579568     2.329746
H      9.031083    14.146737     1.388782

LB-6
   53
xyz
 C     -0.000056    -2.073297     0.000069
 N     -0.687048     0.190211    -0.187307
 C     -1.040532    -1.177788    -0.225043
 N      0.687024     0.190195     0.187316
 C     -1.462672     1.120817     0.587709
 C      1.040456    -1.177812     0.225106
 C      1.462700     1.120736    -0.587727
 N     -2.341376    -1.477854    -0.445182
 C     -2.759859    -2.879539    -0.488389
 C     -3.316813    -0.586322    -1.075617
 N      2.341300    -1.477888     0.445219
 C      2.759767    -2.879575     0.488515
 C      3.316768    -0.586315     1.075545
 C      1.905160     0.784858    -1.866857
 C      1.757719     2.365765    -0.042108
 C      2.657099     1.700304    -2.595981
 C      2.956382     2.951378    -2.053794
 C      2.502733     3.284679    -0.779364
 C     -1.757642     2.365838     0.042044
 C     -1.905119     0.785015     1.866863
 C     -2.502608     3.284814     0.779273
 C     -2.956253     2.951585     2.053723
```

```
C      -2.657011      1.700522      2.595959
C      -4.300682     -1.549439     -1.747599
C      -4.243693     -2.786535     -0.844208
C       4.243615     -2.786558      0.844276
C       4.300651     -1.549390      1.747568
H       1.661402     -0.193394     -2.273101
H       3.010044      1.439229     -3.589711
H       3.544200      3.664031     -2.625412
H       2.733668      4.257455     -0.354616
H       1.401985      2.600155      0.956848
H      -1.401913      2.600171     -0.956927
H      -2.733508      4.257582      0.354487
H      -3.544033      3.664286      2.625319
H      -3.009950      1.439504      3.589706
H      -1.661396     -0.193229      2.273145
H      -2.820240      0.084245     -1.785946
H      -3.821710      0.035880     -0.325093
H      -5.303075     -1.121395     -1.838885
H      -3.946537     -1.805469     -2.753181
H      -4.842814     -2.621515      0.059623
H      -4.610389     -3.693157     -1.333445
H      -2.560030     -3.363085      0.471293
H      -2.186504     -3.420958     -1.252009
H       2.559900     -3.363192     -0.471122
H       2.186434     -3.420930      1.252198
H       4.610318     -3.693146      1.333571
H       4.842706     -2.621616     -0.059589
H       3.946539     -1.805336      2.753182
H       5.303051     -1.121349      1.838783
H       2.820226      0.084315      1.785835
H       3.821642      0.035819      0.324949

LA-1_N2
   27
xyz
C      -0.140971      1.443322     -0.962303
C       1.195281      0.851599     -0.476992
C       1.319811     -0.599551     -0.976889
C       0.144445     -1.461629     -0.480538
C      -1.179738     -0.843438     -0.965867
C      -1.333347      0.604880     -0.465782
C       1.268266      0.892702      1.067494
B       0.011926     -0.009294      1.550663
C      -1.399276      0.632345      1.079311
C       0.159748     -1.547651      1.063711
H       2.238533      0.494725      1.398198
H       1.207456      1.936328      1.408562
H       2.019109      1.443623     -0.898163
H       1.341537     -0.607630     -2.075703
H       2.270388     -1.031876     -0.635253
H       0.241053     -2.470468     -0.904205
H       1.097480     -2.017292      1.394240
H      -0.666495     -2.189413      1.402282
H      -2.025822     -1.450938     -0.616154
```

```
H     -1.209104     -0.856663     -2.064445
H     -2.259699      1.026303     -0.879122
H     -0.240497      2.479252     -0.609958
H     -0.149197      1.477063     -2.060806
H     -1.538563      1.668308      1.420702
H     -2.271380      0.054514      1.418025
N      0.019360     -0.015391      3.166213
N      0.024129     -0.019531      4.269194
```

LA–2_N$_2$
```
    17
xyz
C     -1.449409     -0.522306     -0.679060
C     -1.344282     -0.494129      0.649457
C      0.007928     -0.000084      1.195761
C      1.091983     -0.913294      0.594328
C      1.123567     -0.964542     -0.737334
B     -0.048624     -0.000698     -1.306674
C      0.220211      1.485347     -0.717317
C      0.236623      1.406794      0.613248
H      0.032536      0.000111      2.287074
H     -2.124670     -0.787519      1.346698
H     -2.345962     -0.848677     -1.199619
H      0.367512      2.414493     -1.261672
H      0.395567      2.243157      1.288889
H      1.836107     -1.567604     -1.294066
H      1.759499     -1.455846      1.258648
N     -0.084605     -0.000541     -2.875147
N     -0.110083      0.000046     -3.976866
```

LA–3a_N$_2$
```
    17
xyz
C     -1.253819      0.510618     -0.464773
C     -0.187305      1.262044      0.405698
C      1.040418      0.848017     -0.477980
C      1.179439     -0.464305      0.369574
C      0.004705     -0.009002      1.290994
C     -0.999318     -0.784772      0.382041
C      0.185467     -1.307446     -0.502778
B     -0.016741      0.031091     -1.435857
H      0.338493     -2.357946     -0.750404
H     -0.334292      2.276671      0.782958
H      2.140615     -0.849515      0.717597
H     -1.804801     -1.429952      0.740255
H      0.013275     -0.024977      2.382774
H     -2.245881      0.906685     -0.682075
H      1.873835      1.512664     -0.705906
N     -0.028478      0.052474     -2.928392
N     -0.037290      0.068039     -4.038602
```

LA–4_N$_2$
```
     6
xyz
```

23

```
N     -0.805972     -0.286082      0.299059
N      0.147329      0.848829      0.276339
N      0.653745     -0.543837      0.318718
B      0.008819     -0.026400     -0.897527
N      0.020281     -0.065137     -2.322688
N      0.029320     -0.094964     -3.432986
```

LA–5a_N$_2$
```
    35
xyz
 C    -2.414191     -1.262847     -1.416495
 C    -1.312319     -0.687717     -0.796450
 C    -1.251153     -0.654159      0.608041
 C    -2.278061     -1.188473      1.372675
 C    -3.383448     -1.765456      0.740206
 C    -3.451523     -1.802676     -0.648523
 B     0.020939      0.006903     -1.372783
 C     0.081301      1.503695     -0.783057
 C     0.069094      1.421787      0.620720
 C     0.113367      2.571649      1.395709
 C     0.170615      3.822854      0.774415
 C     0.183113      3.912430     -0.613524
 C     0.138419      2.750827     -1.391966
 C     0.004799      0.001440      1.180303
 C     1.206848     -0.759677      0.623185
 C     1.282352     -0.799117     -0.780434
 C     2.338359     -1.467165     -1.387049
 C     3.315794     -2.093722     -0.606446
 C     3.233843     -2.050106      0.781331
 C     2.174376     -1.379937      1.400307
 H     2.109139     -1.345121      2.485659
 H     3.993200     -2.536908      1.386978
 H     4.139647     -2.614796     -1.086585
 H     2.419873     -1.512336     -2.472472
 H     0.103492      2.500282      2.481184
 H     0.205248      4.725302      1.378386
 H     0.227649      4.885348     -1.095414
 H     0.148952      2.841488     -2.477556
 H    -2.223635     -1.158704      2.458774
 H    -4.189356     -2.184716      1.336105
 H    -4.310995     -2.251398     -1.139145
 H    -2.485759     -1.301516     -2.502883
 H    -0.002009     -0.000880      2.274282
 N     0.030230      0.010052     -2.937937
 N     0.036491      0.012091     -4.039200
```

LA–5b_N$_2$
```
    35
xyz
 C    -2.794799     -1.456606     -1.326442
 C    -1.601732     -0.834460     -0.959190
 C    -1.315943     -0.685822      0.419068
 C    -2.213656     -1.154206      1.377261
 C    -3.400450     -1.772991      0.986190
```

```
  C     −3.693133    −1.925334    −0.366168
 Al     −0.028096    −0.013269    −1.753250
  C     −0.005402    −0.002415     0.866193
  C      0.053858     1.468111     0.398635
  C      0.054938     1.770865    −0.983960
  C      0.110546     3.109926    −1.370210
  C      0.163770     4.135290    −0.424382
  C      0.161907     3.824311     0.932472
  C      0.107182     2.492672     1.342486
  C      1.234318    −0.794996     0.397659
  C      1.482506    −0.966336    −0.985152
  C      2.611936    −1.687073    −1.372730
  C      3.483743    −2.231107    −0.427867
  C      3.228518    −2.055592     0.929277
  C      2.105530    −1.338562     1.340536
  H      1.910252    −1.203880     2.402725
  H      3.902663    −2.476059     1.670721
  H      4.358724    −2.789661    −0.750146
  H      2.828958    −1.835172    −2.429370
  H      0.106199     2.254419     2.404434
  H      0.203156     4.617066     1.674660
  H      0.206644     5.172780    −0.745674
  H      0.113116     3.373684    −2.426590
  H     −1.989259    −1.037415     2.435794
  H     −4.094864    −2.135178     1.739587
  H     −4.617763    −2.407450    −0.672871
  H     −3.041870    −1.585127    −2.379034
  H      0.003929     0.001976     1.959894
  N     −0.044969    −0.020543    −3.943407
  N     −0.053832    −0.024919    −5.042675

LA−5c_N₂
    35
xyz
  C     −2.783732    −1.450412    −1.326551
  C     −1.598338    −0.832333    −0.945660
  C     −1.316052    −0.685781     0.428552
  C     −2.216538    −1.155816     1.381200
  C     −3.401118    −1.773401     0.982580
  C     −3.686080    −1.921497    −0.371937
 Ga     −0.027406    −0.012711    −1.711812
  C     −0.005700    −0.002644     0.871656
  C      0.053790     1.467893     0.408840
  C      0.055323     1.767309    −0.969516
  C      0.110817     3.097582    −1.368796
  C      0.163906     4.127169    −0.428312
  C      0.161654     3.824475     0.930446
  C      0.106735     2.495315     1.347444
  C      1.234036    −0.795111     0.407710
  C      1.479906    −0.964139    −0.970888
  C      2.602277    −1.679796    −1.371184
  C      3.477294    −2.226327    −0.431486
  C      3.228387    −2.055912     0.927505
  C      2.107238    −1.340471     1.345514
```

```
H     1.918058    −1.210294     2.409104
H     3.905718    −2.478888     1.664432
H     4.351154    −2.783662    −0.758151
H     2.811227    −1.821907    −2.429146
H     0.105627     2.264844     2.410853
H     0.202786     4.621413     1.667973
H     0.206999     5.162988    −0.754179
H     0.113540     3.351077    −2.426563
H    −1.999230    −1.042975     2.441377
H    −4.099440    −2.137911     1.731070
H    −4.609215    −2.402828    −0.683627
H    −3.021451    −1.573960    −2.380761
H     0.003417     0.001564     1.965038
N    −0.045163    −0.020875    −3.987497
N    −0.053799    −0.025056    −5.086752
```

LA−5d_N₂
```
   34
xyz
C    −1.769666     2.114900    −1.267842
C    −0.997102     1.202653    −0.563605
C    −0.931465     1.138680     0.831881
C    −1.700306     2.060721     1.537082
C    −2.490176     2.993749     0.860126
C    −2.527743     3.024385    −0.531091
S     0.007971    −0.002147    −1.448621
C     1.580758     0.266719    −0.612490
C     1.536179     0.242722     0.785075
C     2.740576     0.447932     1.452835
C     3.921792     0.664984     0.738473
C     3.923612     0.681379    −0.653489
C     2.734480     0.479213    −1.353286
B     0.052250    −0.026513     1.352137
C    −0.473728    −1.446545     0.802095
C    −0.876433    −2.591900     1.483722
C    −1.300581    −3.724135     0.783110
C    −1.330944    −3.734878    −0.608578
C    −0.934243    −2.604244    −1.322005
C    −0.518953    −1.498096    −0.594695
H    −1.787309     2.124910    −2.353478
H    −3.144414     3.752977    −1.046537
H    −3.082228     3.703983     1.428788
H    −1.697260     2.068091     2.624532
H     2.718034     0.488767    −2.438945
H     4.846372     0.850775    −1.198131
H     4.850257     0.822841     1.278266
H     2.779451     0.442173     2.539605
H    −0.951682    −2.595613    −2.407657
H    −1.661995    −4.619306    −1.142477
H    −1.610440    −4.606973     1.333537
H    −0.866624    −2.621914     2.570743
N     0.077390    −0.040507     2.941356
N     0.094864    −0.050242     4.040469
```

LA–5e_N₂
```
    35
xyz
  C      1.175939    −2.316106    −1.296081
  C      0.645190    −1.277044    −0.550329
  C      0.670544    −1.335243     0.853999
  C      1.226806    −2.432345     1.470286
  C      1.764291    −3.484734     0.733012
  C      1.736363    −3.421748    −0.650479
  C     −0.001442    −0.002334    −1.113444
  F      0.000908     0.000729    −2.475683
  B     −0.005870    −0.008831     1.464311
  C     −1.492520     0.071768     0.853867
  C     −1.429004     0.072042    −0.550494
  C     −2.594104     0.135922    −1.296178
  C     −3.831972     0.200120    −0.650522
  C     −3.900801     0.200170     0.732962
  C     −2.720892     0.135454     1.470199
  F     −2.604313     0.139976    −2.628239
  F     −4.950442     0.261595    −1.367950
  F     −5.080956     0.261447     1.343684
  F     −2.813602     0.136894     2.815257
  F      1.265646    −2.516545     2.815349
  F      2.298642    −4.538817     1.343663
  F      2.245870    −4.419269    −1.367977
  F      1.183642    −2.323571    −2.628148
  C      0.807508     1.241513     0.860746
  C      1.476601     2.270269     1.482706
  C      2.122759     3.263674     0.750883
  C      2.088742     3.211373    −0.632909
  C      1.414486     2.174800    −1.284243
  C      0.776465     1.193779    −0.543901
  F      1.523799     2.342845     2.828178
  F      1.423469     2.188664    −2.616260
  F      2.701256     4.153140    −1.345209
  F      2.765521     4.251987     1.366990
  N     −0.008596    −0.013053     3.052839
  N     −0.010500    −0.016025     4.150432
```

LA–5f_N₂
```
    34
xyz
  C     −1.764116     2.102126    −1.264798
  C     −0.997895     1.188958    −0.557455
  C     −0.956506     1.139632     0.842349
  C     −1.731894     2.063479     1.511957
  C     −2.517940     3.000380     0.832554
  C     −2.536389     3.022563    −0.557607
  S      0.002710    −0.003444    −1.439259
  C      1.546787     0.262890    −0.575848
  C      1.500994     0.245300     0.824542
  C      2.697014     0.451848     1.480189
  C      3.892807     0.667502     0.786780
  C      3.903762     0.678862    −0.603594
```

```
C     2.711753     0.473297    -1.296880
B     0.017065    -0.020431     1.412246
C    -0.502132    -1.435929     0.824654
C    -0.912632    -2.578208     1.480180
C    -1.332080    -3.718538     0.786635
C    -1.345262    -3.727207    -0.603755
C    -0.936476    -2.588703    -1.296943
C    -0.527499    -1.477867    -0.575766
F    -1.773236     2.112929    -2.589493
F    -3.276165     3.904220    -1.200799
F    -3.243684     3.865127     1.509324
F    -1.753388     2.088776     2.848807
F     2.709073     0.481883    -2.621621
F     5.028998     0.881940    -1.260017
F     5.012941     0.860693     1.450470
F     2.746079     0.451473     2.816560
F    -0.944425    -2.584452    -2.621693
F    -1.739992    -4.800260    -1.260271
F    -1.716157    -4.788425     1.450202
F    -0.920734    -2.626957     2.816532
N     0.025738    -0.030160     3.007836
N     0.031694    -0.036932     4.105216
```

LA–5g_N₂
```
    35
xyz
C     0.723230     1.106883    -0.696673
C     0.781363     1.184279     0.723356
C     1.478759     2.254844     1.275569
C     2.104791     3.227425     0.475319
C     2.033164     3.129164    -0.910170
C     1.336679     2.060026    -1.503106
B    -0.033893    -0.078837     1.440253
C    -1.549569    -0.062752     0.909807
C    -1.494166     0.099011    -0.479572
C    -2.635104     0.593477    -1.134725
C    -3.878328     0.553368    -0.480438
C    -3.963435     0.137032     0.849793
C    -2.780306    -0.103361     1.555326
C    -0.085115    -0.136204    -1.120654
Cl   -0.392256    -0.595488    -2.826207
Cl   -2.582577     1.442447    -2.647408
Cl   -5.316098     1.034810    -1.310403
Cl   -5.498715     0.000036     1.626572
Cl   -2.897447    -0.492673     3.250715
Cl    1.627477     2.468369     3.002175
Cl    2.962007     4.543089     1.197363
Cl    2.800246     4.321021    -1.895742
Cl    1.290703     2.004028    -3.232929
C     0.709379    -1.329891    -0.491605
C     1.621204    -2.166558    -1.157965
C     2.096825    -3.321182    -0.513012
C     1.761739    -3.575310     0.818603
C     1.065013    -2.596734     1.534369
```

```
 C      0.594996    −1.453375     0.898089
Cl      2.363166    −1.764818    −2.674478
Cl      0.770341    −2.870823     3.230731
Cl      2.269036    −5.036685     1.584290
Cl      3.116434    −4.433368    −1.356364
 N      0.035520     0.015050     3.025525
 N      0.083084     0.079801     4.119681
```

LA−8a_N$_2$
```
     6
xyz
 B      0.061005    −0.061559    −0.036963
 H     −0.104374     0.262414     1.113428
 H      1.198826     0.001848    −0.431898
 H     −0.777062     0.332883    −0.809423
 N     −0.205684    −1.617082    −0.000679
 N     −0.390455    −2.703560     0.022847
```

LA−8f_N$_2$
```
    15
xyz
 C      1.599973     0.012980     0.109954
 F      2.213026     0.878106     0.957207
 B     −0.019646    −0.007140     0.335292
 C     −0.761913    −1.359347    −0.208251
 F     −0.400671    −2.452474     0.510650
 C     −0.776487     1.386623    −0.063482
 F     −1.000605     1.453509    −1.384618
 F      2.174337    −1.190350     0.325112
 F      1.909211     0.389012    −1.140236
 F     −1.977725     1.499777     0.558149
 F     −0.071547     2.484919     0.284012
 F     −2.108101    −1.287411    −0.127245
 F     −0.448094    −1.600872    −1.490147
 N     −0.186392    −0.093120     1.943288
 N     −0.299221    −0.151567     3.033748
```

LA−4_N$_2$_LB−1
```
    15
xyz
 N     −1.073179    −0.200946    −0.548328
 N     −0.446578     1.135351    −0.890711
 N      0.244251     0.271869     0.034518
 B      0.123752    −0.145804    −1.388631
 N      0.953643    −0.635504    −2.465378
 N      0.545850    −1.620084    −3.091588
 N      0.175631    −3.761103    −4.622728
 H      2.028936    −4.232186    −6.317346
 C      1.240500    −2.996353    −4.894131
 N      1.497300    −1.960766    −4.119992
 H     −0.425373    −3.449475    −3.866109
 N      2.024521    −3.289967    −5.955276
 H      2.331864    −1.381229    −4.184107
 H      2.861256    −2.750581    −6.120672
```

```
H      −0.216753     −4.360382     −5.332270
```

LA−4_N₂_LB−2
```
    40
xyz
 N     −0.764525     −1.596426     −1.131219
 N     −0.019070     −0.296121     −0.840970
 N      0.632674     −1.651590     −1.084628
 B     −0.000118     −0.839765     −2.194656
 N      0.050018     −0.865435     −3.608491
 N      0.144026      0.236571     −4.255863
 H      1.941957     −3.787253     −8.654840
 H      2.044277      2.881193     −9.426810
 H     −3.959256      0.199557     −8.685900
 C      1.503975      2.829544     −8.486537
 C      2.126279     −3.092351     −7.841267
 C     −3.415604     −0.346463     −7.920963
 H      1.589056      0.682424     −8.389870
 H      0.188391     −2.170661     −7.998640
 H     −1.736594      0.998102     −7.954110
 H      4.103354     −3.837820     −7.438652
 H      1.284405      4.962699     −8.310667
 H     −4.949048     −1.832811     −7.664758
 C      1.077365      3.997890     −7.856921
 C     −3.969727     −1.487906     −7.346106
 C      3.339442     −3.119186     −7.156765
 C     −2.162757      0.102597     −7.510786
 C      1.244984      1.592230     −7.904914
 C      1.140446     −2.179815     −7.475040
 C      3.573122     −2.235491     −6.103731
 C      0.394408      3.933728     −6.643441
 C     −3.275586     −2.186198     −6.357980
 C      1.378540     −1.288597     −6.424697
 C      0.553826      1.528189     −6.690585
 C     −1.464986     −0.601787     −6.525169
 C     −2.022340     −1.749450     −5.943956
 C      0.128328      2.700856     −6.055072
 C      2.596111     −1.317828     −5.734757
 H     −3.712534     −3.069573     −5.903016
 H      0.072556      4.845011     −6.149035
 H      4.512640     −2.267560     −5.561186
 P      0.153179     −0.056816     −5.945142
 H     −1.484455     −2.282730     −5.164631
 H     −0.387438      2.645321     −5.101323
 H      2.772051     −0.641604     −4.903154
```

LA−4_N₂_LB−3
```
    46
xyz
 N     −1.921209     −1.017106     −1.338775
 N     −1.686077      0.462216     −1.081533
 N     −0.598511     −0.545825     −1.444240
 B     −1.603423     −0.044212     −2.448406
 N     −1.736803     −0.058949     −3.862575
```

```
N    −2.197710     0.974715    −4.454188
H     0.396782     0.046714    −5.071437
H    −3.007839     3.273766    −4.753390
H    −4.060091    −1.086340    −4.430931
H    −0.611731     3.098268    −5.683154
H    −5.085625     1.134348    −5.075145
H    −1.073733    −1.910640    −5.543445
C    −3.336528     3.370650    −5.789813
C     0.429791     0.286536    −6.136275
C    −4.042090    −1.395030    −5.478477
P    −2.352730     0.754780    −6.156384
H    −3.229537    −2.107939    −5.601571
H    −4.392346     3.110656    −5.845086
H     0.645265     1.347891    −6.248713
H    −3.247834     4.422329    −6.086640
H    −4.980192    −1.922592    −5.688736
H     1.269474    −0.264154    −6.576518
C    −1.047309     3.181583    −6.683315
C    −5.173970     0.709652    −6.078966
C    −0.963643    −1.691403    −6.607406
C    −2.449536     2.544197    −6.749845
C    −0.853755    −0.174196    −6.862260
C    −3.972060    −0.185504    −6.435704
H    −6.071337     0.080462    −6.091889
H    −1.153648     4.248968    −6.907269
H    −0.027492    −2.147684    −6.950568
H    −5.336105     1.513628    −6.800201
H    −1.771763    −2.164931    −7.168374
H    −0.351394     2.769638    −7.416407
C    −4.121714    −0.659270    −7.892223
C    −0.706246     0.060215    −8.376900
C    −2.996045     2.670468    −8.181604
H    −4.043443     2.367238    −8.255238
H    −0.450909     1.093370    −8.623554
H    −3.393355    −1.426716    −8.162365
H    −2.946485     3.725780    −8.474449
H    −5.116919    −1.105395    −8.005400
H     0.116660    −0.568396    −8.737172
H    −4.046833     0.157729    −8.615182
H    −2.419370     2.100527    −8.914567
H    −1.600333    −0.220582    −8.940721
```

LA−4_N$_2$_LB−4
```
   39
xyz
 N    −1.249052    −0.719034    −2.089644
 N    −1.656524    −1.177955    −0.691896
 N    −1.933408    −2.023133    −1.873412
 B    −0.536746    −1.806564    −1.401304
 N     0.634852    −2.691789    −1.406520
 N     1.333513    −2.513148    −2.404502
 H     2.446861    −7.087946    −5.280317
 H     3.137389    −6.083631    −6.579183
 H     1.473139    −5.798985    −6.029837
```

```
C    2.474832   −6.077185   −5.703270
H   −0.986588   −5.115653   −4.883918
H    3.085988   −3.469171   −6.818496
H    0.343371   −5.679739   −3.855529
C   −0.215999   −4.796147   −4.175429
H    4.253731   −2.145849   −6.633653
C    3.230088   −2.465364   −6.410481
N    2.970039   −5.134495   −4.707412
H   −0.802633   −2.875876   −5.982430
H    4.560095   −6.295287   −3.970482
N    0.668758   −3.829836   −4.846955
H    2.533250   −1.784200   −6.915731
H    5.005591   −5.160653   −5.273040
C    4.384521   −5.293008   −4.377160
C   −0.053788   −2.605528   −5.231667
H   −0.703020   −4.338931   −3.304477
P    2.221351   −3.724914   −4.289748
H    0.629312   −1.877956   −5.670469
N    3.032414   −2.461665   −4.963094
H    4.695394   −4.556259   −3.633464
H   −0.549080   −2.147441   −4.367799
C    3.222240   −1.159206   −4.321362
H    4.155639   −0.732208   −4.702322
H    3.050275   −5.434915   −2.061948
N    2.325597   −3.554295   −2.625172
H    2.392921   −0.476219   −4.538054
C    2.347901   −4.684280   −1.698008
H    1.353902   −5.126051   −1.569819
H    3.301224   −1.276565   −3.242475
H    2.680693   −4.318579   −0.724612

LA−4_N₂_LB−5
    41
xyz
N    1.626728    4.468028   −2.009031
N    2.763568    4.789725   −1.238019
N    2.430067    3.314311   −1.429758
B    2.979964    4.077882   −2.547472
N    3.700567    4.331729   −3.747475
N    4.327868    3.373626   −4.314902
H    6.573426    6.516826   −8.784979
H    8.392296    3.741585   −8.486760
H    5.458718    3.655238  −10.055143
N    6.409459    4.457006   −8.346510
C    6.651078    5.818818   −7.936107
C    7.403913    3.441340   −8.102967
C    5.218050    4.129881   −9.090199
H    7.679569    5.887170   −7.563455
H    7.113837    2.538429   −8.652391
H    4.689656    5.062118   −9.319885
C    5.678705    6.265048   −6.832675
C    7.535648    3.111554   −6.607802
C    4.291383    3.198767   −8.293583
H    5.933997    7.268498   −6.476267
```

```
H     8.239835     2.285937    −6.459403
H     3.357400     3.023197    −8.838209
H     7.951145     3.978136    −6.081327
H     4.663999     6.327606    −7.240581
H     4.772724     2.222266    −8.172660
N     5.690680     5.366593    −5.683594
N     6.270889     2.731671    −5.985209
N     3.947511     3.734419    −6.980665
H     2.588904     5.232593    −7.611858
H     7.436549     6.110430    −4.757800
H     6.029973     0.774805    −6.771578
C     6.415624     5.807054    −4.492312
C     2.668117     4.436159    −6.860384
C     6.010696     1.303465    −5.808725
P     5.069130     3.844001    −5.769872
H     1.841370     3.731808    −6.998319
H     5.893643     6.644128    −4.018829
H     6.768497     0.868346    −5.149214
H     6.477364     4.996989    −3.763073
H     2.572206     4.886488    −5.869609
H     5.035974     1.158421    −5.340342


LA−4_N₂_LB−6
    59
xyz
N    −5.823145     0.063378    −0.356230
N    −5.714267    −1.314659     0.234873
N    −5.717470    −1.062445    −1.268071
B    −4.548357    −0.712527    −0.423786
N    −3.140188    −0.379975    −0.522660
N    −2.380861    −0.795896     0.393598
H     2.691113    −2.511118    −3.676419
C     2.938707    −2.096970    −2.703775
H     5.046615    −2.493118    −2.893738
H    −2.227422     3.782285    −2.148968
C     4.262876    −2.084814    −2.262647
H     0.896317    −1.571012    −2.230296
C     1.931587    −1.574691    −1.898977
C    −1.744758     4.120261    −1.225577
H     0.014054     2.907855    −1.797566
H    −1.467779     5.170939    −1.344067
C    −0.531137     3.246371    −0.910891
C     4.581770    −1.549870    −1.016265
H    −3.200785     1.795997    −0.474930
H    −3.701400     4.141432    −0.211374
C     2.260434    −1.055946    −0.648469
C    −2.662144     3.860948    −0.027593
H     2.882074     2.025740    −1.357919
C    −2.523760     2.354874     0.177236
H    −1.740627    −3.280886    −0.039930
N    −1.123826     2.092958    −0.212064
H     5.612234    −1.538023    −0.674321
C    −0.522542     0.909784    −0.084076
C     3.575800    −1.033776    −0.201769
```

```
N      0.864205      0.820631     -0.179710
H     -0.332710     -5.238856      0.197972
C     -1.043820     -0.353257      0.249693
H      0.168363      3.779763     -0.257498
C      2.750373      2.351028     -0.330489
C      0.056913     -1.201522      0.431600
N      1.232733     -0.502317      0.198952
C     -1.131434     -3.335290      0.863544
N      0.085257     -2.503892      0.717011
H      1.897515     -3.529021      0.308572
H     -2.305690      4.411671      0.851371
C     -0.562558     -4.725593      1.138986
C      1.715939      1.813463      0.425244
H      4.401289      3.729141     -0.342376
H     -2.696757      2.027281      1.205560
C      3.592131      3.302478      0.242518
C      1.291639     -3.217382      1.167156
H      3.798467     -0.618485      0.776437
H     -1.267028     -5.344195      1.699490
H     -1.738254     -2.966455      1.694470
C      0.726739     -4.428313      1.908864
H      1.430653     -5.264314      1.918640
H      1.902311     -2.563468      1.797599
C      1.512426      2.202761      1.747420
C      3.388576      3.709940      1.559109
H      0.699182      1.764086      2.319692
C      2.349019      3.160155      2.311236
H      0.495231     -4.162100      2.946455
H      4.039558      4.457788      2.002039
H      2.191552      3.477407      3.337680
```

LA−5a_N₂_LB−1
```
   44
xyz
C      1.222624     -2.103448     -1.639858
C      0.659523     -1.232606     -0.717075
C      0.772491     -1.456796      0.666274
C      1.468233     -2.582015      1.098266
C      2.040202     -3.467183      0.177324
C      1.918383     -3.229713     -1.189001
C     -0.119859      0.026739     -1.086420
H     -0.182973      0.162627     -2.171400
B      0.029571     -0.296616      1.514731
N      0.142213     -0.501543      3.059937
N     -0.453445      0.322795      3.711957
N     -0.295445      0.064680      5.171291
C     -0.932628      0.869258      5.997254
N     -0.753727      0.798145      7.334494
H      1.570422     -2.777471      2.164841
H      2.581546     -4.342966      0.528525
H      2.362371     -3.916617     -1.905278
H      1.124461     -1.912336     -2.707209
C      0.685339      1.097683      0.988062
C      1.301524      2.134521      1.681986
```

```
C      1.800223     3.255558     1.007343
C      1.681620     3.346228    −0.375788
C      1.063980     2.313390    −1.088588
C      0.575781     1.204765    −0.411175
H      1.406159     2.081428     2.765576
H      0.967270     2.379232    −2.170898
H      2.068410     4.214823    −0.902781
H      2.284741     4.054650     1.564316
C     −1.496072    −0.265447     0.944179
C     −1.502760    −0.094322    −0.453274
C     −2.692047    −0.038735    −1.166755
C     −3.912335    −0.158715    −0.493975
C     −3.924660    −0.333331     0.886041
C     −2.719444    −0.384949     1.597008
H     −2.675587     0.096611    −2.246803
H     −4.845902    −0.118492    −1.049481
H     −4.871523    −0.434869     1.412131
H     −2.752132    −0.529372     2.677027
N     −1.771164     1.782945     5.490954
H     −1.453704     1.184769     7.950456
H     −1.810167     1.851438     4.477826
H      0.272344    −0.731439     5.451648
H     −0.172864     0.069973     7.722173
H     −2.039768     2.587432     6.036031
```

LA−5a_N₂_LB−2
```
   69
xyz
C      3.287275    −1.940247     1.794407
C      3.350361    −2.559787     3.037879
C      2.580860    −2.078241     4.096567
C      1.748880    −0.974392     3.919879
C      1.683988    −0.341549     2.683148
C      2.462135    −0.822848     1.619933
P      2.235393    −0.061198     0.018705
C      3.168721    −0.920434    −1.252073
C      2.616816    −2.082210    −1.805436
C      3.323875    −2.781984    −2.777550
C      4.573015    −2.324747    −3.195734
C      5.118976    −1.164954    −2.648214
C      4.417449    −0.457350    −1.676387
N      0.545433    −0.062877    −0.548229
N     −0.274902    −0.408449     0.304685
B     −1.761819    −0.236227    −0.039017
C     −2.723771    −1.140453     0.898432
C     −2.398400    −2.111655     1.841178
C     −3.401586    −2.784466     2.548344
C     −4.741533    −2.486132     2.315310
C     −5.084089    −1.509161     1.374789
C     −4.080718    −0.848263     0.679448
H     −1.352615    −2.348785     2.033972
H     −3.135506    −3.543356     3.281132
H     −5.521470    −3.009259     2.863150
H     −6.130225    −1.269127     1.191921
```

```
C    −4.322454    0.243473    −0.359154
C    −3.661740   −0.209809    −1.659181
C    −2.280255   −0.465906    −1.562290
C    −1.608432   −0.878739    −2.710299
C    −2.288203   −1.041891    −3.923064
C    −3.653827   −0.786765    −3.998833
C    −4.344197   −0.366384    −2.857904
H    −5.412606   −0.163596    −2.909833
H    −4.183400   −0.911092    −4.940134
H    −1.746524   −1.364948    −4.809557
H    −0.537138   −1.068403    −2.675262
C    −3.573931    1.486711     0.111545
C    −4.165961    2.723914     0.323802
C    −3.385443    3.806943     0.742887
C    −2.018853    3.639079     0.940238
C    −1.428306    2.388636     0.720531
C    −2.192466    1.302241     0.306846
H    −5.234880    2.852287     0.162783
H    −0.354614    2.281292     0.874421
H    −1.408451    4.478430     1.266643
H    −3.847969    4.776070     0.911995
H    −5.390203    0.444194    −0.498046
C     2.671959    1.680670     0.069234
C     2.053730    2.550886    −0.838418
C     2.362104    3.906703    −0.802251
C     3.282936    4.390894     0.125466
C     3.897890    3.523200     1.027020
C     3.592710    2.165819     1.004486
H     1.137861   −0.611420     4.740058
H     2.894839   −3.678598    −3.213649
H     1.871332    4.585370    −1.492553
H     2.625187   −2.570988     5.063415
H     3.516410    5.451220     0.151971
H     5.119964   −2.870938    −3.958544
H     1.318394    2.176167    −1.544468
H     1.636540   −2.430223    −1.490029
H     1.024266    0.509561     2.545730
H     6.087574   −0.806583    −2.982777
H     3.995612   −3.421395     3.178849
H     4.608266    3.903896     1.754434
H     3.876254   −2.323118     0.965612
H     4.055678    1.491528     1.720071
H     4.834817    0.455381    −1.259470
```

LA−5a_N$_2$_LB−3
```
   75
xyz
C    −3.244238   −1.470789    −0.458911
C    −1.856380   −1.457657    −0.225231
C    −1.152122   −2.648977    −0.358869
C    −1.805975   −3.837205    −0.705580
C    −3.179197   −3.835614    −0.926795
C    −3.900667   −2.643304    −0.806537
B    −1.344388    0.047017     0.147328
```

N	0.146988	0.066899	0.510878
N	0.942246	−0.030438	−0.440195
P	2.635476	0.018862	0.051273
C	2.895029	−0.813297	1.736303
C	4.372026	−1.196860	1.941809
H	−0.074758	−2.668010	−0.198077
H	−1.240796	−4.761688	−0.802300
H	−3.691368	−4.755732	−1.196265
H	−4.973834	−2.634664	−0.988817
C	−3.927386	−0.113488	−0.326531
C	−3.229280	0.832347	−1.301090
C	−1.838301	0.950079	−1.115756
C	−1.133090	1.788132	−1.973587
C	−1.784770	2.502376	−2.985563
C	−3.160204	2.376372	−3.151227
C	−3.885653	1.533303	−2.303559
H	−4.961749	1.427538	−2.429891
H	−3.670340	2.927551	−3.937144
H	−1.215412	3.153534	−3.645499
H	−0.053512	1.884292	−1.870169
C	−3.646856	0.402332	1.081131
C	−4.626527	0.749360	2.001266
C	−4.250831	1.214674	3.265648
C	−2.901540	1.325872	3.589603
C	−1.924172	0.972180	2.652295
C	−2.279837	0.506068	1.389888
H	−5.680336	0.660937	1.742349
H	−0.871411	1.064715	2.917719
H	−2.608363	1.689041	4.572322
H	−5.011968	1.488949	3.991841
H	−5.001561	−0.180977	−0.529511
C	2.007668	−2.073601	1.842385
C	2.454263	0.107503	2.891964
C	3.460791	−0.903275	−1.372602
C	4.974697	−0.645678	−1.448178
C	2.801016	−0.496632	−2.711859
C	3.207222	−2.415825	−1.216384
C	3.058529	1.860817	0.075513
C	4.426519	2.117644	0.732924
C	1.950728	2.634036	0.824442
C	3.088749	2.431796	−1.354815
H	0.946426	−1.817817	1.818159
H	1.714764	−0.603898	−2.681667
H	0.995111	2.590175	0.296242
H	3.194103	−1.167367	−3.484669
H	2.217252	−2.538177	2.813176
H	2.258912	3.685238	0.868314
H	2.204764	−2.822707	1.077137
H	3.041215	0.519976	−3.018913
H	1.783863	2.296805	1.845684
H	2.138814	−2.644370	−1.153702
H	1.405627	0.393368	2.790573
H	2.168461	2.220584	−1.905030
H	2.557127	−0.465387	3.821132

```
H     3.593575    −2.913466    −2.112829
H     3.177418     3.521061    −1.272570
H     4.657281     3.184955     0.635056
H     5.386157    −1.259314    −2.258204
H     4.480199    −1.589626     2.959730
H     4.703172    −1.982400     1.258687
H     4.434876     1.882959     1.799145
H     5.207881     0.395475    −1.685106
H     3.944957     2.081590    −1.935355
H     3.073008     1.000534     2.997699
H     3.722855    −2.854066    −0.359845
H     5.236775     1.563008     0.250701
H     5.503182    −0.917074    −0.530638
H     5.051522    −0.344927     1.847399
```

LA−5a_N₂_LB−5
```
   70
xyz
C     3.608588     1.213073     0.840424
C     2.216709     1.069072     0.992539
C     1.551286     1.945035     1.843571
C     2.248497     2.937310     2.542882
C     3.625463     3.062471     2.387038
C     4.308115     2.196408     1.526681
B     1.656381    −0.164032     0.085172
N     0.154809    −0.439888     0.227219
N    −0.599912     0.503299    −0.089356
P    −2.278020     0.112152     0.020986
N    −2.580944    −0.967042     1.225440
C    −1.947843    −0.818172     2.536605
H     0.469883     1.875314     1.961824
H     1.713617     3.613358     3.206722
H     4.170057     3.832528     2.927699
H     5.384294     2.294845     1.394586
C     4.250692     0.227383    −0.132432
C     3.538251     0.396094    −1.471982
C     2.143109     0.215484    −1.424274
C     1.415852     0.376293    −2.599131
C     2.055376     0.696166    −3.802697
C     3.436239     0.864043    −3.834918
C     4.180800     0.716658    −2.660091
H     5.260516     0.855198    −2.677594
H     3.936094     1.113505    −4.767567
H     1.472696     0.817646    −4.713605
H     0.331545     0.268374    −2.587538
C     3.936539    −1.177237     0.373086
C     4.892856    −2.135062     0.681740
C     4.485364    −3.393025     1.137869
C     3.128484    −3.672610     1.277785
C     2.174488    −2.697699     0.963120
C     2.562884    −1.440563     0.508141
H     5.952535    −1.910810     0.570242
H     1.114616    −2.924980     1.075476
H     2.811556    −4.651308     1.632383
```

```
H      5.227709    −4.149082     1.381838
H      5.329051     0.396199    −0.224901
C     −3.617285    −1.985058     1.089239
C     −5.026494    −1.372263     1.065345
N     −5.127571    −0.344623     0.056629
C     −5.169194    −0.711132    −1.338463
C     −3.963850    −0.125869    −2.089495
N     −2.696161    −0.484869    −1.462391
C     −1.974660    −1.631925    −2.019719
C     −5.410686     1.016409     0.444623
C     −4.195168     1.660093     1.128777
N     −2.979745     1.574826     0.323812
C     −2.586823     2.765569    −0.433993
H     −6.279366     1.078935     1.119236
H     −6.099813    −0.377524    −1.824382
H     −5.768809    −2.171347     0.911979
H     −5.666768     1.585784    −0.455919
H     −5.147741    −1.804358    −1.409187
H     −5.241878    −0.920500     2.040222
H     −4.383819     2.718190     1.336831
H     −3.937899    −0.478498    −3.125687
H     −3.511776    −2.685987     1.923451
H     −4.051768     0.965471    −2.129534
H     −4.021711     1.173050     2.095224
H     −3.450241    −2.561598     0.172621
H     −2.711154    −0.700815     3.316554
H     −3.380180     3.069084    −1.130321
H     −2.616865    −2.521795    −2.048063
H     −1.324668    −1.689976     2.756565
H     −2.383263     3.589362     0.257097
H     −1.637611    −1.400933    −3.035106
H     −1.672111     2.565868    −0.994193
H     −1.302404     0.061919     2.553204
H     −1.094810    −1.860835    −1.413883

LA−5a_N₂_LB−6
    88
xyz
C      5.142168     2.751047     2.078559
C      4.078015     1.970563     1.639812
C      4.052576     1.533551     0.317004
C      5.079698     1.850403    −0.563440
C      6.148871     2.624285    −0.116024
C      6.177433     3.077692     1.200946
N      2.959732     0.726581    −0.159937
C      1.638625     1.097929     0.065008
C      0.904734    −0.031337     0.461361
C      1.822422    −1.085847     0.580910
N      3.089405    −0.643909     0.214394
N      1.277676     2.378983    −0.011677
C      1.977604     3.388256    −0.822209
C      0.899382     4.448274    −1.044077
C      0.111978     4.406051     0.269002
C      0.031246     2.910171     0.566885
```

```
N    −0.490545    −0.236426     0.592455
N    −1.173571     0.403345    −0.234540
B    −2.686781     0.154308    −0.152068
C    −3.126659    −1.269960    −0.812459
C    −2.349420    −2.268340    −1.393146
C    −2.933955    −3.434877    −1.901416
C    −4.313299    −3.607299    −1.835427
C    −5.111509    −2.606132    −1.271024
C    −4.521638    −1.452682    −0.772109
H    −1.269843    −2.136174    −1.472520
H    −2.311984    −4.203992    −2.355748
H    −4.771995    −4.511264    −2.228695
H    −6.192309    −2.731081    −1.227124
C    −5.294375    −0.291827    −0.152654
C    −4.936866     0.962201    −0.947174
C    −3.558922     1.243784    −0.989736
C    −3.141264     2.354406    −1.719214
C    −4.065453     3.178357    −2.373057
C    −5.425682     2.890405    −2.306487
C    −5.863491     1.770050    −1.591789
H    −6.925386     1.533217    −1.545231
H    −6.146170     3.527890    −2.813314
H    −3.721800     4.041791    −2.939669
H    −2.076997     2.576577    −1.800499
N     1.611218    −2.354624     0.922722
C     0.286205    −2.880453     1.334211
C     0.574483    −4.353115     1.608137
C     2.013126    −4.339262     2.129540
C     2.692626    −3.306247     1.230751
C     3.873088    −1.400448    −0.733425
C     3.293950    −1.849985    −1.918251
C     4.068723    −2.568731    −2.822589
C     5.413458    −2.819857    −2.546001
C     5.985420    −2.352517    −1.364512
C     5.211797    −1.640385    −0.450110
C    −4.756783    −0.093561     1.260462
C    −5.548528    −0.126990     2.401009
C    −4.965740     0.078366     3.655164
C    −3.596779     0.313088     3.746922
C    −2.808577     0.339439     2.590337
C    −3.370496     0.138947     1.331255
H    −6.618965    −0.309634     2.319167
H    −1.736732     0.507276     2.682233
H    −3.138415     0.473647     4.720927
H    −5.580177     0.054964     4.552023
H    −6.373950    −0.478914    −0.153110
H     3.623636    −2.930881    −3.744301
H     6.015340    −3.381155    −3.254470
H     0.252843     4.159248    −1.879848
H     2.246711    −1.641520    −2.122409
H     2.349839     2.934258    −1.745511
H     1.330356     5.428932    −1.261612
H    −0.827308     2.445579     0.072870
H    −0.884504     4.845328     0.184843
```

```
H      5.029425      1.494556     −1.587972
H     −0.459590     −2.715270      0.557506
H      7.032134     −2.546102     −1.150390
H      0.509626     −4.931088      0.678952
H      2.828979      3.808035     −0.273449
H      3.068282     −3.766951      0.310108
H      0.658626      4.936547      1.057913
H      6.954379      2.877718     −0.798539
H     −0.017996      2.669816      1.633109
H      5.632909     −1.272996      0.480863
H     −0.139306     −4.775422      2.318783
H     −0.054597     −2.352451      2.230481
H      2.507305     −5.312560      2.074030
H      3.524074     −2.786528      1.716978
H      3.264373      1.706334      2.310245
H      2.034265     −4.003513      3.172705
H      7.006663      3.687871      1.546345
H      5.165607      3.104238      3.105088

LA−5b_N₂_LB−5
    70
xyz
  C      3.885937      1.407649      0.226846
  C      2.624149      1.572656      0.845108
  C      2.373103      2.785145      1.491388
  C      3.323990      3.808460      1.537775
  C      4.560406      3.626386      0.925301
  C      4.838008      2.425629      0.270524
 Al      1.632132     −0.106327      0.512980
  N     −0.259341     −0.333841      0.996018
  N     −0.929881      0.404715      0.256806
  P     −2.666503      0.115722      0.240322
  N     −3.239422     −0.426274      1.686721
  C     −2.849476      0.237374      2.929679
  H      1.411000      2.947857      1.978007
  H      3.101249      4.741891      2.050521
  H      5.309553      4.414013      0.955337
  H      5.805930      2.285554     −0.208742
  C      4.210977      0.094150     −0.507966
  C      3.259621     −0.116518     −1.697603
  C      1.875477     −0.244870     −1.449171
  C      1.031510     −0.405477     −2.549588
  C      1.523770     −0.454112     −3.857430
  C      2.893041     −0.335045     −4.079975
  C      3.759110     −0.162295     −2.998431
  H      4.828868     −0.060925     −3.176078
  H      3.289290     −0.371229     −5.091991
  H      0.844437     −0.580839     −4.698495
  H     −0.046592     −0.484426     −2.392262
  C      4.174613     −1.107638      0.451568
  C      5.328646     −1.863442      0.655205
  C      5.311559     −2.958719      1.519743
  C      4.134787     −3.296929      2.181774
  C      2.981310     −2.535463      1.974047
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C     2.968810    −1.433347     1.115110
H     6.250288    −1.599813     0.138145
H     2.070735    −2.815723     2.503681
H     4.115093    −4.149134     2.857860
H     6.215831    −3.542729     1.673964
H     5.229877     0.176616    −0.902448
C    −4.326686    −1.398977     1.751924
C    −5.652121    −0.818856     1.232641
N    −5.486440    −0.257372    −0.087031
C    −5.333608    −1.133891    −1.224254
C    −3.975826    −0.900338    −1.903982
N    −2.870140    −1.002833    −0.957191
C    −2.141612    −2.274040    −0.910833
C    −5.731010     1.149019    −0.302424
C    −4.603468     1.997605     0.304252
N    −3.280048     1.594279    −0.163970
C    −2.689090     2.375117    −1.256304
H    −6.695574     1.469948     0.121693
H    −6.141899    −0.999429    −1.960040
H    −6.425186    −1.602964     1.252037
H    −5.783004     1.329087    −1.381897
H    −5.391723    −2.170019    −0.872672
H    −5.989123    −0.023060     1.906423
H    −4.736700     3.055777     0.057542
H    −3.803415    −1.628839    −2.702541
H    −4.424722    −1.725573     2.792183
H    −3.963762     0.089720    −2.372812
H    −4.637710     1.920954     1.397052
H    −4.057803    −2.285505     1.167074
H    −3.717653     0.711764     3.405850
H    −3.360570     2.401987    −2.124814
H    −2.840037    −3.112828    −0.797175
H    −2.405346    −0.486946     3.618735
H    −2.503233     3.398555    −0.916673
H    −1.559771    −2.407625    −1.828228
H    −1.733516     1.941797    −1.555768
H    −2.104042     1.009676     2.729861
H    −1.449594    −2.287281    −0.065899

LA−5b_N₂_LB−6
     88
xyz
C     6.113979     1.660093     2.029455
C     4.833490     1.308365     1.615949
C     4.631899     0.887539     0.303103
C     5.690761     0.797560    −0.592227
C     6.973545     1.141359    −0.169936
C     7.183783     1.576556     1.136768
N     3.313689     0.521499    −0.146544
C     2.222578     1.349402     0.083492
C     1.142794     0.580150     0.544556
C     1.617198    −0.747435     0.662781
N     2.945603    −0.799747     0.249287
N     2.341053     2.667957    −0.060909
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```
C     3.355564     3.324683    −0.898936
C     2.727716     4.689286    −1.177727
C     1.980960     4.986822     0.126461
C     1.377295     3.631209     0.495999
N    −0.251964     0.810104     0.640474
N    −0.770780     1.682987    −0.094248
Al   −2.608989     1.041545    −0.070628
C    −2.624275    −0.602624    −1.206404
C    −1.660076    −1.261457    −1.973734
C    −1.920502    −2.480419    −2.607681
C    −3.180466    −3.061165    −2.483056
C    −4.166863    −2.421391    −1.728779
C    −3.893531    −1.208255    −1.097378
H    −0.670174    −0.812410    −2.082785
H    −1.150685    −2.970997    −3.201688
H    −3.399780    −4.007006    −2.973075
H    −5.151321    −2.877541    −1.632400
C    −4.956447    −0.521396    −0.227204
C    −5.274095     0.897306    −0.730707
C    −4.263568     1.889185    −0.757438
C    −4.618484     3.156630    −1.228222
C    −5.914396     3.452577    −1.658960
C    −6.893256     2.464048    −1.623682
C    −6.569375     1.188857    −1.159513
H    −7.336897     0.416352    −1.132781
H    −7.906077     2.680580    −1.955211
H    −6.158093     4.449696    −2.019750
H    −3.867318     3.945480    −1.265035
N     0.979783    −1.848052     1.032539
C    −0.454158    −1.901010     1.424456
C    −0.686291    −3.381433     1.699262
C     0.671936    −3.866339     2.209788
C     1.655673    −3.130889     1.300923
C     3.353203    −1.790907    −0.720016
C     2.568755    −2.030653    −1.846322
C     2.981110    −2.984608    −2.770455
C     4.176021    −3.677968    −2.573641
C     4.958395    −3.420888    −1.449561
C     4.544437    −2.475381    −0.513332
C    −4.493047    −0.515285     1.238328
C    −5.194427    −1.250667     2.194254
C    −4.760561    −1.278040     3.520598
C    −3.621340    −0.565532     3.887779
C    −2.924676     0.167467     2.922496
C    −3.333827     0.212186     1.586932
H    −6.085233    −1.808043     1.907126
H    −2.030987     0.714814     3.225030
H    −3.280509    −0.577362     4.921503
H    −5.313646    −1.850376     4.261833
H    −5.878460    −1.111107    −0.287682
H     2.368030    −3.186961    −3.643314
H     4.494703    −4.422561    −3.296982
H     2.020333     4.615111    −2.010735
H     1.636899    −1.488900    −1.986119
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H      3.540938      2.729471     −1.797834
H      3.480275      5.441459     −1.427709
H      0.397424      3.460845      0.034682
H      1.209769      5.752008      0.012421
H      5.500413      0.465126     −1.608135
H     −1.086559     −1.511381      0.629836
H      5.886976     −3.962041     −1.294941
H     −0.956020     −3.895824      0.769717
H      4.300604      3.434077     −0.353864
H      1.811324     −3.679690      0.365491
H      2.685024      5.324099      0.896493
H      7.805884      1.074817     −0.863969
H      1.280612      3.473998      1.575036
H      5.130604     −2.268469      0.376967
H     −1.499482     −3.523864      2.414328
H     −0.612767     −1.284086      2.312871
H      0.801933     −4.950055      2.150061
H      2.631949     −2.950519      1.761390
H      3.990177      1.363669      2.299500
H      0.819201     −3.559596      3.251951
H      8.182523      1.851646      1.462471
H      6.279004      1.996996      3.048440

LA−5d_N₂_LB−1
    43
xyz
  C    −1.574523      2.099460     −1.845979
  C    −0.885993      1.365516     −0.888593
  C    −0.928812      1.603361      0.487695
  C    −1.744402      2.663174      0.889297
  C    −2.456825      3.423973     −0.040054
  C    −2.374396      3.150674     −1.403689
  S     0.144378     −0.015375     −1.405457
  C     1.651570      0.403616     −0.517482
  C     1.491506      0.685888      0.841662
  C     2.664778      0.991808      1.534134
  C     3.903696      1.012927      0.890162
  C     4.009129      0.730905     −0.470107
  C     2.862923      0.417390     −1.197013
  B    −0.037683      0.589589      1.407465
  C    −0.553214     −0.910215      1.045193
  C    −1.048050     −1.877692      1.921332
  C    −1.454400     −3.129398      1.455581
  C    −1.378365     −3.451388      0.100983
  C    −0.890060     −2.512792     −0.805249
  C    −0.497102     −1.280491     −0.298244
  H    −1.497487      1.863714     −2.903460
  H    −2.931179      3.746220     −2.119788
  H    −3.088343      4.237921      0.304740
  H    −1.838540      2.902033      1.945383
  H     2.919800      0.189297     −2.257445
  H     4.975442      0.749092     −0.963454
  H     4.799337      1.247984      1.458303
  H     2.622552      1.211008      2.597805
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```
H    −0.821558    −2.740896    −1.864960
H    −1.696832    −4.427292    −0.250878
H    −1.835947    −3.865037     2.157912
H    −1.116325    −1.648935     2.981230
N    −0.161162     0.852094     2.932770
N     0.201539     1.954325     3.305968
N     0.276219     3.424985     6.610026
H     0.963632     4.051435     3.519065
C     0.403172     3.251895     5.289064
N     0.048048     2.097158     4.726506
H    −0.086445     2.693908     7.203764
N     0.883421     4.222817     4.514453
H     1.167755     5.115899     4.886721
H    −0.327692     1.301268     5.237940
H     0.538319     4.291135     7.057180
```

LA−5d_N₂_LB−2
```
    68
xyz
C     2.546434     2.142990    −1.623753
C     3.057681     3.373185    −2.022240
C     4.023688     4.013981    −1.246652
C     4.483293     3.429877    −0.067425
C     3.977709     2.200550     0.344209
C     3.008043     1.558776    −0.435098
P     2.342718    −0.029606     0.057277
C     3.023031    −1.365074    −0.926178
C     4.152584    −1.171294    −1.726419
C     4.651576    −2.233979    −2.475245
C     4.024760    −3.477091    −2.426373
C     2.895163    −3.668746    −1.629360
C     2.389929    −2.615148    −0.877419
N     0.633925     0.069483    −0.435060
N    −0.178349    −0.205595     0.451391
B    −1.669423    −0.079418     0.070448
C    −2.597749    −0.613665     1.294435
C    −2.170404    −1.153886     2.509435
C    −3.091791    −1.572687     3.470764
C    −4.464445    −1.462145     3.247918
C    −4.928990    −0.925089     2.049363
C    −3.977450    −0.522467     1.120480
H    −1.104553    −1.243924     2.703223
H    −2.736513    −1.991610     4.408157
H    −5.171902    −1.791075     4.002326
H    −5.993119    −0.827311     1.854707
S    −4.488597     0.187591    −0.451674
C    −3.498484    −0.826254    −1.562217
C    −2.136771    −0.901541    −1.258375
C    −1.366853    −1.676862    −2.127806
C    −1.943958    −2.331562    −3.217341
C    −3.309334    −2.227967    −3.476348
C    −4.111209    −1.457938    −2.637247
H    −0.296107    −1.764645    −1.967003
H    −1.318492    −2.927587    −3.876023
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45

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H    −3.749370    −2.738788    −4.326679
H    −5.177060    −1.357587    −2.820977
C    −3.470814     1.672706    −0.441019
C    −4.057353     2.907499    −0.687427
C    −3.231098     4.029290    −0.679443
C    −1.867652     3.877779    −0.435239
C    −1.316630     2.617369    −0.196312
C    −2.111580     1.470010    −0.189808
H    −5.122230     3.000228    −0.880551
H    −0.246618     2.536547    −0.021792
H    −1.224113     4.753076    −0.431396
H    −3.651616     5.012324    −0.864837
C     2.554947    −0.322723     1.808305
C     3.292738    −1.412411     2.284233
C     3.398455    −1.622606     3.655911
C     2.764385    −0.757201     4.545103
C     2.023283     0.325520     4.070930
C     1.914644     0.546696     2.703666
H     5.234514     3.931642     0.534058
H     5.528230    −2.088810    −3.098288
H     3.976981    −2.461656     4.028901
H     4.419977     4.974029    −1.563053
H     2.847960    −0.926267     5.614388
H     4.416112    −4.302092    −3.013655
H     3.786783    −2.089241     1.593363
H     4.637134    −0.199959    −1.770185
H     4.331158     1.749518     1.267231
H     2.408046    −4.638097    −1.595467
H     2.700903     3.831796    −2.938989
H     1.527370     0.995209     4.766209
H     1.789569     1.646146    −2.223529
H     1.333711     1.388628     2.337693
H     1.509433    −2.765350    −0.256825

LA−5d_N₂_LB−3
    74
xyz
C     3.099624    −0.729020     1.523164
C     1.730410    −0.788332     1.247624
C     0.962842    −1.480155     2.185660
C     1.542411    −2.073015     3.308657
C     2.914118    −1.987155     3.535866
C     3.717119    −1.299433     2.629171
B     1.257890    −0.057472    −0.135940
N    −0.240843    −0.150875    −0.499787
N    −1.038721     0.108642     0.414056
P    −2.749962    −0.023730    −0.046057
C    −3.162410    −1.855030     0.187301
C    −2.068372    −2.724295    −0.468976
H    −0.111435    −1.548410     2.048086
H     0.915152    −2.606187     4.017595
H     3.358208    −2.448144     4.412066
H     4.788721    −1.215007     2.785324
S     4.098377     0.168584     0.324586
```

```
C      3.121936      1.674916      0.216870
C      1.753229      1.492665      0.002824
C      0.991300      2.660212     −0.048356
C      1.578460      3.918590      0.095845
C      2.949867      4.048415      0.302465
C      3.745310      2.906626      0.370333
H     −0.081967      2.594673     −0.200895
H      0.958087      4.809113      0.047167
H      3.399994      5.029382      0.414207
H      4.815643      2.981841      0.539239
C      3.541806     −0.648714     −1.176705
C      4.469049     −1.157016     −2.077694
C      3.975641     −1.787818     −3.217566
C      2.598198     −1.886502     −3.409994
C      1.703445     −1.359602     −2.477120
C      2.156988     −0.717945     −1.323046
H      5.537830     −1.069567     −1.905008
H      0.634492     −1.449049     −2.648456
H      2.217824     −2.381432     −4.299132
H      4.663998     −2.199681     −3.948406
C     −4.539807     −2.188106     −0.417137
C     −3.184322     −2.232050      1.680543
C     −3.020443      0.572407     −1.827444
C     −2.135639      1.805249     −2.114324
C     −4.501396      0.929774     −2.057835
C     −2.603520     −0.497168     −2.856245
C     −3.553531      1.087473      1.250346
C     −2.886488      0.863644      2.627867
C     −5.066950      0.837511      1.370083
C     −3.307270      2.565965      0.889893
H     −5.342291     −1.568203     −0.008473
H     −5.180303      0.101912     −1.836847
H     −5.603395      0.976491      0.428583
H     −4.625710      1.176881     −3.118129
H     −4.775198     −3.229084     −0.168931
H     −5.474473      1.558636      2.087327
H     −4.558508     −2.106187     −1.505182
H     −4.820629      1.804159     −1.487184
H     −5.296187     −0.158727      1.755527
H     −3.227024     −1.392072     −2.832609
H     −4.034072     −1.804364      2.215824
H     −3.828416      2.885124     −0.014041
H     −3.280665     −3.321548      1.742365
H     −2.720984     −0.053135     −3.851170
H     −3.692357      3.177232      1.712973
H     −3.300831      1.612122      3.312347
H     −2.378142      2.151909     −3.125170
H     −2.382942     −3.769799     −0.376317
H     −1.913264     −2.522147     −1.527131
H     −3.100353     −0.112688      3.059127
H     −2.305640      2.643017     −1.439540
H     −2.240448      2.791224      0.794166
H     −2.261247     −1.957482      2.196907
H     −1.555026     −0.775457     −2.738770
```

```
H      −1.804139       1.000447       2.588083
H      −1.074504       1.547607      −2.101171
H      −1.106540      −2.624367       0.040519
```

LA−5d_N₂_LB−4
```
     67
xyz
 C       5.021230      −0.888198       1.703021
 C       3.897388      −0.508777       0.979095
 C       2.590110      −0.514403       1.463501
 C       2.434422      −0.938066       2.784931
 C       3.534870      −1.329431       3.549115
 C       4.824036      −1.307579       3.016634
 S       4.070201       0.051146      −0.722521
 C       2.821853      −0.992617      −1.492056
 C       1.565573      −0.980573      −0.880177
 C       0.610483      −1.811245      −1.471919
 C       0.908113      −2.585032      −2.594667
 C       2.176691      −2.553901      −3.170640
 C       3.161233      −1.743332      −2.611059
 B       1.420243      −0.025625       0.441745
 C       1.866091       1.468926      −0.045556
 C       1.137646       2.656956       0.049017
 C       1.660014       3.866347      −0.413011
 C       2.928961       3.926215      −0.986837
 C       3.689671       2.764215      −1.095851
 C       3.132978       1.583462      −0.620394
 H       6.016042      −0.859873       1.267796
 H       5.673175      −1.613015       3.619530
 H       3.387616      −1.654896       4.575145
 H       1.438326      −0.955471       3.218916
 H       4.160041      −1.704950      −3.036330
 H       2.402068      −3.157271      −4.044007
 H       0.141868      −3.223982      −3.026230
 H      −0.387701      −1.854074      −1.048610
 H       4.682961       2.786441      −1.534961
 H       3.328555       4.870264      −1.342848
 H       1.073002       4.775989      −0.319884
 H       0.148099       2.643008       0.498557
 N       0.049589      −0.004183       1.153554
 N      −0.913403       0.116678       0.407809
 H      −5.589638      −2.736999       0.216873
 H      −4.947141      −2.581178      −1.435059
 H      −5.791931      −1.212778      −0.675837
 C      −5.115367      −2.048663      −0.491008
 H      −6.601544       0.134093       1.638048
 H      −3.328491      −1.148830      −2.400830
 H      −5.138967      −0.704856       2.186999
 C      −5.539749       0.261872       1.876341
 H      −1.728320      −0.379619      −2.568805
 C      −2.806769      −0.195040      −2.488981
 N      −3.848300      −1.571625       0.065369
 H      −6.385924       2.082182       0.256592
 H      −3.289376      −3.417270       0.872935
```

```
N     −4.835026      0.761084      0.694323
H     −3.156577      0.300547     −3.399612
H     −2.525690     −3.045309     −0.691559
C     −2.848343     −2.619517      0.266899
C     −5.292241      2.069755      0.228266
H     −5.452736      0.967766      2.710936
P     −3.478514      0.028217      0.120939
H     −4.982839      2.239432     −0.803036
N     −3.094454      0.669204     −1.342323
H     −1.974229     −2.231722      0.791031
H     −4.916947      2.880450      0.864800
C     −2.425632      1.972438     −1.430088
H     −1.348031      1.835793     −1.573955
H     −1.956855     −0.804666      2.930634
N     −2.159573      0.258408      1.106539
H     −2.843322      2.532048     −2.273552
C     −2.171154      0.204888      2.561776
H     −3.142965      0.537380      2.927259
H     −2.577043      2.552891     −0.517595
H     −1.396697      0.875823      2.939195
```

LA−5d_N$_2$_LB−5
```
   69
xyz
  C      4.010562     −0.364289      2.891090
  C      3.395285     −0.204970      1.655631
  C      2.023236     −0.029152      1.460630
  C      1.245168     −0.026436      2.619931
  C      1.823902     −0.178115      3.881136
  C      3.200186     −0.344719      4.023804
  S      4.394762     −0.239629      0.158490
  C      3.442787     −1.438707     −0.788593
  C      2.068196     −1.198951     −0.856448
  C      1.326546     −2.142677     −1.569325
  C      1.941159     −3.238407     −2.177828
  C      3.318494     −3.430325     −2.086241
  C      4.093162     −2.517894     −1.373881
  B      1.545112      0.145411     −0.090958
  C      2.418612      1.379727     −0.696492
  C      1.933642      2.546172     −1.292461
  C      2.805558      3.526373     −1.769206
  C      4.187929      3.370621     −1.665115
  C      4.710557      2.221335     −1.076538
  C      3.805644      1.272840     −0.615977
  H      5.084919     −0.500327      2.975684
  H      3.641906     −0.463472      5.007877
  H      1.192860     −0.170553      4.765621
  H      0.166862      0.081021      2.541619
  H      5.167352     −2.650015     −1.281390
  H      3.788510     −4.285432     −2.561072
  H      1.337707     −3.954599     −2.728632
  H      0.247487     −2.034661     −1.641469
  H      5.783275      2.077924     −0.983967
  H      4.857411      4.138541     −2.039156
```

```
H     2.404291     4.425501    −2.228665
H     0.859279     2.684641    −1.381861
N     0.041322     0.428325    −0.269170
N    −0.724947    −0.446555     0.169239
H    −6.213076     0.511883     1.715116
H    −5.903884     1.978173    −1.114607
H    −6.347399    −1.196217    −0.985843
N    −5.115762     0.289234    −0.092666
C    −5.263039     0.810773     1.249344
C    −5.116143     1.216541    −1.204281
C    −5.462792    −1.094116    −0.340817
H    −5.257946     1.904919     1.202974
H    −5.311611     0.658590    −2.126117
H    −5.704740    −1.571888     0.614381
C    −4.080257     0.325798     2.098355
C    −3.738388     1.887554    −1.294790
C    −4.260852    −1.801418    −0.979649
H    −4.073663     0.798377     3.084836
H    −3.646909     2.488922    −2.203847
H    −4.434656    −2.877483    −1.068968
H    −3.599709     2.570117    −0.449496
H    −4.159177    −0.754067     2.263821
H    −4.103482    −1.418992    −1.994359
N    −2.803267     0.620125     1.447590
N    −2.666157     0.892975    −1.301122
N    −3.037902    −1.607541    −0.198632
H    −3.466054    −2.932691     1.404841
H    −2.791055     2.719488     1.769237
H    −2.837340     0.363631    −3.340592
C    −2.124303     1.852908     1.859067
C    −2.653823    −2.698844     0.704839
C    −2.060105     0.577864    −2.596760
P    −2.428659    −0.086421    −0.000442
H    −2.422597    −3.592179     0.117441
H    −1.799070     1.764107     2.900197
H    −1.448231     1.417311    −2.939021
H    −1.244890     2.032350     1.236708
H    −1.762194    −2.423979     1.268984
H    −1.414603    −0.298480    −2.517923
```

LA−5d_N2_LB−6
```
   87
xyz
C     4.770773    −2.438218    −2.077443
C     4.288005    −1.424395    −1.258654
C     2.942638    −1.080740    −1.115618
C     2.046562    −1.824780    −1.887742
C     2.488298    −2.850591    −2.724621
C     3.843325    −3.165577    −2.819680
S     5.443895    −0.430173    −0.300016
C     4.870326     1.208216    −0.778894
C     3.495223     1.404554    −0.657157
C     3.028008     2.660530    −1.052602
C     3.903065     3.642128    −1.520523
```

```
C      5.273301      3.397678     −1.613085
C      5.777784      2.153774     −1.240576
B      2.610878      0.152877     −0.094449
C      3.292721     −0.261163      1.334329
C      2.682750     −0.351583      2.588607
C      3.410487     −0.700338      3.727048
C      4.775063     −0.977471      3.650778
C      5.421343     −0.903536      2.419858
C      4.658700     −0.547636      1.313443
H      5.832805     −2.657233     −2.142466
H      4.179179     −3.964684     −3.472742
H      1.768095     −3.408661     −3.317332
H      0.985278     −1.593472     −1.842572
H      6.839716      1.936452     −1.312245
H      5.946138      4.166858     −1.978586
H      3.513307      4.610563     −1.822309
H      1.961211      2.864436     −1.006431
H      6.483145     −1.115717      2.332092
H      5.333177     −1.249789      4.540844
H      2.906883     −0.759868      4.688149
H      1.617384     −0.159318      2.677186
N      1.118651      0.512201     −0.034617
N      0.402857     −0.378343      0.471926
H     −3.272687      3.131295     −3.755889
C     −3.765620      2.829229     −2.837037
H     −5.605815      3.844237     −3.302511
H     −1.055984     −4.464768     −1.709216
C     −5.077673      3.228520     −2.580983
H     −2.064752      1.715907     −2.104506
C     −3.085805      2.038276     −1.915885
C     −1.690865     −4.597757     −0.825721
H     −2.273705     −5.512216     −0.957410
H     −2.925039     −2.921844     −1.564892
C     −5.712064      2.840499     −1.402235
C     −2.586517     −3.376078     −0.629076
H      0.378735     −2.820596      0.081126
H      0.069639     −5.199163      0.353879
C     −0.837340     −4.597444      0.445079
C     −3.726566      1.668054     −0.735557
H     −5.140521     −1.040904     −1.725075
C     −0.512068     −3.117573      0.639901
H      0.742808      2.365535      0.932037
N     −1.709866     −2.439578      0.098415
H     −6.733293      3.150594     −1.204178
C     −1.906010     −1.124175      0.174143
C     −5.033792      2.058342     −0.470440
N     −3.127722     −0.554767     −0.094224
C     −0.981209     −0.108134      0.490808
H      0.118202      4.695414      1.126474
H     −3.467276     −3.628482     −0.028924
C     −5.348862     −1.343878     −0.703504
C     −1.720954      1.093329      0.574804
N     −3.043909      0.831646      0.227055
C     −0.069546      2.600804      1.619939
```

```
N    −1.369261    2.306832    0.988743
H    −2.550834    3.933915    0.323590
H    −1.418044   −4.981215    1.291691
C    −4.380796   −1.158398    0.275884
C    −0.173365    4.077718    1.983453
H    −7.330740   −2.070556   −1.111685
H    −0.358604   −2.829721    1.682659
C    −2.347808    3.383453    1.248176
C    −6.568386   −1.919600   −0.353907
H    −5.506874    1.751119    0.457396
H     0.477590    4.335293    2.821746
H     0.043194    1.967748    2.510669
C    −1.659733    4.259566    2.294697
H    −3.287708    2.952912    1.603883
H    −1.991905    5.298479    2.234995
C    −4.611684   −1.523534    1.600303
C    −6.805045   −2.303516    0.964532
H    −3.841600   −1.358085    2.349225
C    −5.828206   −2.105399    1.941633
H    −1.883761    3.888711    3.301149
H    −7.753766   −2.757371    1.233974
H    −6.016296   −2.402276    2.968765

LA−5e_N2_LB−1
    44
xyz
C     1.430380    2.259851    1.502719
C     0.768499    1.221069    0.879576
C     0.661865    1.257146   −0.520991
C     1.200740    2.303477   −1.252144
C     1.864139    3.339463   −0.594339
C     1.979919    3.318776    0.784184
B     0.054175   −0.102318    1.527892
C    −1.489111   −0.071635    0.943158
C    −1.487124    0.039036   −0.467029
C    −2.668656    0.083411   −1.189526
C    −3.896203    0.005160   −0.531171
C    −3.922384   −0.135379    0.841579
C    −2.724038   −0.181951    1.550781
C    −0.089984    0.062592   −1.105567
C     0.633249   −1.213641   −0.662326
C     0.728591   −1.352601    0.733309
C     1.331562   −2.486884    1.235815
C     1.856397   −3.468282    0.397493
C     1.766697   −3.311618   −0.974774
C     1.148567   −2.180817   −1.509740
F     1.088441   −2.098218   −2.842623
F     2.266659   −4.247259   −1.785914
F     2.439415   −4.557897    0.905315
F     1.428978   −2.705916    2.562613
F    −2.713887    0.197134   −2.519347
F    −5.035972    0.051947   −1.223146
F    −5.091578   −0.230501    1.484081
F    −2.872084   −0.376046    2.891258
```

```
F     1.123344     2.385333    -2.583451
F     2.386611     4.350523    -1.291795
F     2.614496     4.311643     1.414556
F     1.579978     2.307652     2.845973
F    -0.167174     0.141401    -2.468584
N     0.345047    -0.139297     3.040145
N    -0.493372     0.363675     3.759715
N    -2.254977     0.764063     5.683518
H    -1.324393     0.730275     8.076641
C    -0.982229     0.629311     6.054881
N    -0.066588     0.351811     5.136430
H    -2.487143     0.618498     4.703300
N    -0.631536     0.775695     7.345072
H     0.868261     0.002380     5.336769
H     0.338137     0.747456     7.621141
H    -2.928485     1.213980     6.283685
```

LA-5e_N₂_LB-2
```
    69
xyz
C     3.212751    -2.697848    -0.914586
C     2.642922    -1.489656    -0.546414
C     1.268388    -1.391365    -0.262773
C     0.517753    -2.547177    -0.336190
C     1.072467    -3.770240    -0.704211
C     2.421549    -3.843912    -0.997983
C     3.399776    -0.170097    -0.390108
F     4.732243    -0.325875    -0.655932
B     0.829165     0.139869     0.132348
C     1.385168     1.077865    -1.090393
C     2.755369     0.851700    -1.333928
C     3.433873     1.553195    -2.317642
C     2.764427     2.515423    -3.073606
C     1.431096     2.778967    -2.822200
C     0.764438     2.065916    -1.828056
F     4.728574     1.367523    -2.593222
F     3.412392     3.192705    -4.024473
F     0.792997     3.720197    -3.525301
F    -0.519436     2.424543    -1.609756
F    -0.805316    -2.566506    -0.041284
F     0.312523    -4.868129    -0.770664
F     2.964694    -5.010594    -1.352560
F     4.509627    -2.840956    -1.200863
C     1.816978     0.513432     1.372926
C     1.509903     0.980637     2.634072
C     2.502201     1.249932     3.574878
C     3.830570     1.052064     3.241425
C     4.169898     0.590498     1.968826
C     3.172323     0.326541     1.044686
F     0.237112     1.209382     3.014168
F     5.472108     0.427411     1.713121
F     4.787642     1.307540     4.137751
F     2.182643     1.699078     4.792782
N    -0.665810     0.173229     0.506664
```
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```
N    -1.469662     0.188478    -0.422956
H    -2.165912    -2.015654     4.395181
H    -3.485528     4.911185    -0.518477
H    -3.464335    -2.851142    -3.828081
C    -3.788785    -2.695333    -2.804069
C    -2.720504    -1.230648     3.891160
C    -3.961965     3.954463    -0.706971
H    -3.520437    -0.406809     5.709650
H    -4.949732    -4.505121    -2.727708
H    -5.630320     4.809210    -1.762253
H    -2.697770    -0.852874    -2.585819
H    -2.414203     2.832157     0.275726
H    -2.053067    -1.821646     1.935276
C    -4.622595    -3.624537    -2.182943
C    -5.165563     3.893702    -1.408517
C    -3.479647    -0.322947     4.627705
C    -3.359029     2.785210    -0.258199
C    -2.655395    -1.122996     2.507186
C    -3.359789    -1.570255    -2.109756
C    -4.179021     0.697336     3.985551
C    -5.032411    -3.433014    -0.865066
C    -5.770602     2.665098    -1.666881
C    -3.770652    -1.381548    -0.783511
C    -3.968514     1.551542    -0.517448
C    -3.363217    -0.099254     1.861373
C    -5.173084     1.488572    -1.224364
C    -4.607171    -2.311531    -0.159199
C    -4.118600     0.817445     2.601175
H    -6.704406     2.621107    -2.218658
H    -4.766808     1.404377     4.562525
H    -5.677707    -4.160196    -0.382211
P    -3.172055     0.063643     0.091192
H    -4.655683     1.618904     2.102295
H    -4.915804    -2.168351     0.872442
H    -5.637041     0.528953    -1.435074
```

LA−5e_N₂_LB−3
```
    75
xyz
C     3.639650     1.377856    -1.872268
C     2.733917     0.730817    -1.047270
C     1.348010     0.907956    -1.208586
C     0.925839     1.778276    -2.191296
C     1.819711     2.437856    -3.031584
C     3.178322     2.231188    -2.875151
C     3.103343    -0.187150     0.120058
F     4.459565    -0.306278     0.246891
B     0.470749     0.056343    -0.120708
C     1.071028     0.587428     1.320576
C     2.472608     0.411201     1.385607
C     3.196638     0.794334     2.503189
C     2.548001     1.381339     3.589722
C     1.185099     1.593065     3.534186
C     0.473388     1.203435     2.400954
```

```
F      4.519362      0.638573      2.612275
F      3.241721      1.749206      4.668646
F      0.555655      2.175584      4.559598
F     −0.845100      1.498163      2.423586
F     −0.383708      2.059838     −2.377602
F      1.375731      3.269747     −3.978489
F      4.045133      2.856492     −3.674852
F      4.963954      1.236229     −1.764331
C      1.046703     −1.478410     −0.246156
C      0.374876     −2.670273     −0.419164
C      1.030253     −3.896857     −0.485280
C      2.406948     −3.937759     −0.369058
C      3.119151     −2.753269     −0.180342
C      2.446204     −1.543393     −0.118183
F     −0.973529     −2.718278     −0.528421
F      4.445293     −2.862023     −0.065587
F      3.048964     −5.105531     −0.431406
F      0.337550     −5.026950     −0.656860
N     −1.032474      0.080052     −0.484615
N     −1.861389     −0.016484      0.424320
H     −1.989421     −1.214632     −2.317442
H     −2.539121     −1.565076      2.290774
H     −1.995974      2.605631      0.460555
C     −2.960456      2.780901     −0.019508
C     −3.594426     −1.315912      2.415874
C     −3.054568     −1.429870     −2.406190
H     −4.064549     −2.098262      3.023294
H     −3.291210     −1.558228     −3.469184
H     −3.285776      3.792736      0.248594
H     −3.260295     −2.376600     −1.910866
H     −3.655354     −0.384323      2.975491
H     −2.813813      2.757720     −1.097643
H     −3.113469     −2.908997      0.226907
H     −2.440272      1.219761     −2.592456
H     −3.087077      1.620770      2.472761
C     −4.336290     −1.281114      1.060931
C     −4.034692      1.798361      0.497028
C     −3.907489     −0.250948     −1.891107
C     −4.159614     −2.679988      0.439141
C     −3.493524      0.972554     −2.730740
C     −4.036350      1.927419      2.032555
H     −3.633268      0.704839     −3.784638
H     −4.511214     −3.412551      1.174506
H     −4.177472      2.988433      2.268774
P     −3.574100      0.044636     −0.047410
H     −5.661970      3.193253      0.390115
H     −6.231997     −1.872954      1.878573
H     −5.543357     −0.627901     −3.224949
C     −5.837664     −1.033385      1.294493
C     −5.398080     −0.549170     −2.141025
C     −5.422785      2.208346     −0.027191
H     −5.717959     −1.498618     −1.706174
H     −5.456862      2.303964     −1.113964
H     −6.032584     −0.124559      1.867183
```

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H   -4.853578    1.382268    2.509001
H   -4.106443    1.856113   -2.544082
H   -4.752196   -2.826677   -0.465793
H   -6.213973    1.521734    0.286772
H   -6.411178   -0.986157    0.364980
H   -6.062653    0.240143   -1.780676
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LA−5e_N₂_LB−4
```
    68
xyz
 C    2.452699    1.869669   -2.301741
 C    2.085911    1.024351   -1.266556
 C    0.826334    1.133935   -0.642267
 C    0.004470    2.158505   -1.065599
 C    0.351918    3.013366   -2.109017
 C    1.574746    2.863784   -2.734664
 C    2.986158   -0.060336   -0.665765
 F    4.206301   -0.094103   -1.283864
 B    0.628928    0.015167    0.546979
 C    1.902965    0.294630    1.523868
 C    3.128175    0.239414    0.833105
 C    4.327182    0.449390    1.494725
 C    4.325040    0.722426    2.862991
 C    3.127974    0.786130    3.554205
 C    1.929967    0.573083    2.874766
 F    5.519531    0.406575    0.889998
 F    5.478232    0.925629    3.506618
 F    3.131058    1.053177    4.863810
 F    0.798835    0.659744    3.602473
 F   -1.187043    2.419820   -0.475563
 F   -0.489177    3.978608   -2.502361
 F    1.918679    3.677139   -3.736489
 F    3.629159    1.795120   -2.931277
 C    1.002043   -1.418893   -0.162952
 C    0.292681   -2.603648   -0.195739
 C    0.763295   -3.729758   -0.867248
 C    1.986103   -3.679564   -1.510998
 C    2.739690   -2.506288   -1.474844
 C    2.253540   -1.394969   -0.805051
 F   -0.898231   -2.749060    0.431672
 F    3.917221   -2.527597   -2.106613
 F    2.445006   -4.753879   -2.158217
 F    0.041742   -4.856500   -0.891615
 N   -0.731036   -0.061303    1.267991
 N   -1.688850   -0.044270    0.524410
 H   -4.437338    3.191860    1.710232
 H   -3.696046    3.260432    0.087988
 H   -3.001846    2.212305    1.333789
 C   -3.935944    2.605173    0.932941
 H   -5.925006   -1.711836    2.588686
 H   -3.145569   -2.249619   -0.888794
 H   -5.938658    0.059385    2.424283
 C   -6.206781   -0.878255    1.933536
 H   -2.020863   -1.234012   -1.790418
```

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C    -3.078738    -1.489145    -1.668100
N    -4.823617     1.517768     0.518980
H    -5.331929    -3.078448     0.332710
H    -6.660345     2.467362     0.871033
N    -5.554349    -0.980972     0.630163
H    -3.473377    -1.900612    -2.603697
H    -6.039139     2.656345    -0.785148
C    -6.136417     1.956602     0.054926
C    -5.853068    -2.211968    -0.095109
H    -7.293896    -0.894079     1.793928
P    -4.270741    -0.008406     0.251448
H    -5.585099    -2.108928    -1.146755
N    -3.847783    -0.290358    -1.311784
H    -6.733734     1.101361    -0.265372
H    -6.931569    -2.391163    -0.037873
C    -3.613144     0.824950    -2.230902
H    -2.553561     1.103706    -2.234473
H    -1.962312    -0.497294     2.982116
N    -2.958046    -0.284010     1.207330
H    -3.912594     0.516423    -3.237525
C    -3.005451    -0.463870     2.649955
H    -3.495167    -1.405721     2.909999
H    -4.204711     1.696728    -1.949199
H    -3.504924     0.373757     3.150285
```

LA–5e_N₂_LB–5
```
    70
xyz
C     3.965241    -0.307502     2.211633
C     3.008318    -0.167213     1.219748
C     1.635939    -0.264326     1.515116
C     1.273834    -0.509649     2.824447
C     2.223645    -0.652929     3.834167
C     3.568613    -0.550915     3.526862
C     3.303290     0.096976    -0.261335
F     4.649079     0.178726    -0.492689
B     0.699795    -0.064885     0.190794
C     1.279882    -1.182722    -0.860437
C     2.665953    -1.038117    -1.068493
C     3.356472    -1.886317    -1.919475
C     2.680121    -2.912491    -2.578957
C     1.324819    -3.084629    -2.369494
C     0.647135    -2.223306    -1.509794
F     4.668452    -1.785010    -2.154403
F     3.339569    -3.732583    -3.401053
F     0.674233    -4.077212    -2.986682
F    -0.667834    -2.484405    -1.335140
F    -0.017636    -0.627879     3.198557
F     1.846111    -0.888590     5.095232
F     4.485178    -0.687092     4.489260
F     5.280200    -0.222665     1.984007
C     1.201090     1.374322    -0.423936
C     0.495153     2.521902    -0.724558
C     1.107032     3.656034    -1.252755
```

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C      2.470033     3.651284    -1.481230
C      3.217575     2.514219    -1.174896
C      2.591190     1.394651    -0.650882
F     -0.840250     2.626278    -0.514878
F      4.531014     2.578783    -1.412061
F      3.067311     4.733016    -1.986877
F      0.385244     4.745964    -1.536434
N     -0.807129    -0.104975     0.510199
N     -1.566626    -0.045812    -0.467895
H     -7.125414     1.685620    -0.284682
H     -7.180799    -1.579401    -0.593667
H     -6.744812    -0.219203     2.363700
N     -6.080572    -0.040637     0.360454
C     -6.304807     1.019448    -0.593822
C     -6.235654    -1.415141    -0.053066
C     -5.963269     0.273879     1.764999
H     -6.602598     0.568600    -1.547114
H     -6.268877    -2.044126     0.843548
H     -6.100385     1.353902     1.889387
C     -5.027484     1.848059    -0.797750
C     -5.056714    -1.847648    -0.939011
C     -4.579407    -0.128311     2.299284
H     -5.162731     2.584402    -1.596066
H     -5.107127    -2.916380    -1.170474
H     -4.444338     0.207426     3.332099
H     -5.099370    -1.314361    -1.894947
H     -4.803841     2.410351     0.115683
H     -4.490229    -1.219385     2.311308
N     -3.877985     1.017333    -1.148259
N     -3.770213    -1.587648    -0.300424
N     -3.502095     0.446732     1.498640
H     -3.590499     2.367027     2.365612
H     -4.335774     0.686595    -3.188049
H     -3.857272    -3.109508     1.172133
C     -3.484322     0.976434    -2.558498
C     -2.839169     1.637967     2.035930
C     -3.155470    -2.693484     0.437710
P     -3.256060    -0.040786    -0.050746
H     -2.197048     1.359819     2.876050
H     -3.123309     1.961395    -2.869970
H     -2.851968    -3.479806    -0.258441
H     -2.675916     0.258649    -2.702147
H     -2.217458     2.108949     1.274362
H     -2.266241    -2.348147     0.969295

LA-5e_N₂_LB-6
    88
xyz
C     -4.468765    -0.356243     2.461993
C     -3.695691    -0.204188     1.321682
C     -2.360350     0.236031     1.395257
C     -1.869717     0.567290     2.644056
C     -2.631532     0.418049     3.800870
C     -3.928687    -0.052723     3.710919
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C    -4.188677    -0.440216    -0.107723
F    -5.500840    -0.830032    -0.126305
B    -1.646341     0.333402    -0.081140
C    -2.652966     1.326111    -0.905410
C    -3.986047     0.868532    -0.886652
C    -4.990662     1.572929    -1.530210
C    -4.687259     2.754448    -2.207941
C    -3.384770     3.218159    -2.234703
C    -2.386360     2.496772    -1.583609
F    -6.270756     1.184391    -1.545489
F    -5.652995     3.438347    -2.829610
F    -3.094391     4.352588    -2.882175
F    -1.138643     3.013614    -1.650500
F    -0.634088     1.085504     2.822081
F    -2.120408     0.733526     4.997110
F    -4.665146    -0.199564     4.816802
F    -5.736655    -0.782876     2.442076
C    -1.928948    -1.127665    -0.787000
C    -1.056152    -1.993415    -1.417167
C    -1.472031    -3.213896    -1.943578
C    -2.804533    -3.573604    -1.864346
C    -3.719832    -2.705393    -1.269247
C    -3.285838    -1.498036    -0.745090
F     0.260878    -1.710652    -1.576592
F    -4.995537    -3.104652    -1.242444
F    -3.212733    -4.742920    -2.366621
F    -0.590637    -4.037512    -2.527007
N    -0.158210     0.699990    -0.107519
N     0.518788    -0.036013     0.636784
H     4.233061    -3.134351    -3.582784
C     4.753015    -2.737529    -2.716286
H     6.636555    -3.646961    -3.226616
H     1.429170     4.302644    -1.879709
C     6.103653    -3.024358    -2.514165
H     3.013211    -1.709813    -1.953740
C     4.065382    -1.939900    -1.807334
C     2.132579     4.569245    -1.084554
H     3.452977     2.946990    -1.803120
H     2.618135     5.512301    -1.348243
C     3.147302     3.446023    -0.878959
C     6.769644    -2.516453    -1.400382
H     0.332972     2.712707     0.188826
H     0.440767     5.118549     0.208649
C     4.739584    -1.449388    -0.690900
C     1.408254     4.615090     0.264189
H     6.020668     1.350399    -1.708717
C     1.244449     3.137013     0.617097
H     0.439106    -2.503671     0.801086
N     2.412215     2.502884    -0.020377
H     7.820553    -2.739625    -1.243212
C     2.700413     1.210718     0.095117
C     6.084428    -1.726951    -0.479250
N     3.984394     0.750125    -0.154257
H     1.298338    -4.747809     1.042186
```

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C    1.910324    0.138007    0.555824
H    4.044041    3.818840   -0.370298
C    6.141793    1.735115   -0.700723
C    2.774350   -0.964683    0.692822
N    4.047499   -0.612001    0.262412
C    1.189252   -2.653003    1.574863
N    2.518128   -2.201823    1.104050
H    3.863612   -3.720085    0.490811
H    2.024123    5.131760    1.010159
C    1.425991   -4.118572    1.930456
C    5.144435    1.506288    0.239098
H    8.056363    2.645472   -1.060977
H    1.253799    2.930812    1.691258
C    7.273264    2.460289   -0.332112
C    3.565790   -3.193654    1.404388
H    6.579347   -1.328456    0.401317
H    0.726798   -4.465545    2.694688
H    0.890384   -2.057506    2.443970
C    2.884678   -4.139780    2.391699
H    3.332379   -5.136449    2.373306
H    4.447418   -2.693949    1.816475
C    5.260130    1.981815    1.543610
C    7.392956    2.952504    0.965708
H    4.467972    1.785702    2.261586
C    6.386822    2.713398    1.903351
H    2.966986   -3.745291    3.410949
H    8.271166    3.524687    1.249463
H    6.481615    3.096584    2.914846
```

LA–5f_N₂_LB–1
```
    43
xyz
C   -0.481424   -1.211931   -0.241372
C   -0.533556   -0.800085    1.094147
C   -0.927289   -1.771451    1.998998
C   -1.271624   -3.064701    1.594465
C   -1.219459   -3.427670    0.253447
C   -0.810396   -2.485091   -0.682653
B   -0.098498    0.755546    1.391629
N   -0.432650    1.136133    2.837665
N    0.259187    1.972475    3.393339
N   -0.248733    2.275541    4.679067
C    0.486725    3.049745    5.483838
N    1.697384    3.428859    5.087768
S    0.085378   -0.001743   -1.425293
C    1.564475    0.525007   -0.567719
C    1.447626    0.856200    0.793228
C    2.655233    1.150504    1.405290
C    3.873377    1.165039    0.719393
C    3.932692    0.856656   -0.631538
C    2.752676    0.518428   -1.282981
C   -0.982212    1.349384   -0.972657
C   -1.697739    2.003340   -1.964754
C   -2.530438    3.055343   -1.602449
```

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C    −2.612702    3.411474   −0.261813
C    −1.873167    2.726561    0.706080
C    −1.032471    1.672429    0.386922
N    −0.002574    3.425186    6.669772
F    −1.600771    1.643502   −3.240379
F    −3.232001    3.707570   −2.515182
F    −3.400452    4.411825    0.096582
F    −2.024064    3.153820    1.967710
F     2.782411    0.190375   −2.570544
F     5.086509    0.869053   −1.278343
F     4.986331    1.472370    1.367187
F     2.749643    1.419940    2.720557
F    −0.739005   −2.813948   −1.968881
F    −1.545194   −4.654258   −0.122736
F    −1.647050   −3.959508    2.492719
F    −0.981670   −1.525323    3.311517
H     2.055022    3.079227    4.205832
H    −0.958093    3.229092    6.930019
H     2.235492    4.112071    5.599153
H    −1.098795    1.796699    4.971045
H     0.568353    3.911496    7.345694
```

LA−5f_N₂_LB−2
```
   68
xyz
  C    −3.218922    2.821278   −1.115541
  C    −2.662086    1.623665   −0.691861
  C    −1.313151    1.443661   −0.363575
  C    −0.536894    2.586991   −0.467746
  C    −1.056153    3.811583   −0.895148
  C    −2.399035    3.937626   −1.225729
  S    −3.723745    0.203574   −0.515056
  C    −2.750426   −0.979072   −1.432171
  C    −1.399419   −1.103513   −1.079207
  C    −0.724634   −2.119691   −1.736864
  C    −1.330989   −2.913073   −2.715170
  C    −2.664787   −2.730268   −3.055079
  C    −3.391907   −1.751694   −2.389056
  B    −0.885806   −0.079864    0.109863
  C    −1.872984   −0.417007    1.379969
  C    −1.534184   −0.829231    2.658500
  C    −2.502907   −1.077060    3.636135
  C    −3.855428   −0.924142    3.354653
  C    −4.235004   −0.524774    2.078621
  C    −3.245044   −0.285770    1.137098
  F    −4.511284    2.917817   −1.411291
  F    −2.887053    5.100193   −1.628532
  F    −0.263397    4.867987   −0.982438
  F     0.766844    2.595097   −0.150658
  F    −4.680379   −1.578341   −2.669561
  F    −3.234873   −3.486885   −3.979854
  F    −0.631058   −3.859283   −3.320831
  F     0.546124   −2.426990   −1.453457
  F    −5.524093   −0.381253    1.783952
```
```
                            61
```

```
F     −4.766278    −1.161731     4.286386
F     −2.134776    −1.465430     4.846467
F     −0.264360    −1.023639     3.022382
N      0.600202    −0.120062     0.513094
N      1.415950    −0.119056    −0.408719
H      5.861535     3.976825    −0.539975
H      6.347967    −2.943930    −2.240522
H      4.641090    −1.202421     4.668848
C      4.086307    −0.504559     4.050046
C      5.181291     3.263720    −0.994383
C      5.475751    −2.904277    −1.596032
H      5.218479     4.214942    −2.922459
H      3.533002     0.762896     5.696193
H      5.301921    −5.040975    −1.432760
H      4.487909    −1.580197     2.234154
H      5.403908    −0.753815    −1.585025
H      4.951180     2.117874     0.811113
C      3.464501     0.601596     4.624694
C      4.886677    −4.081479    −1.140134
C      4.818741     3.395340    −2.333231
C      4.945721    −1.671165    −1.226837
C      4.670463     2.216436    −0.233432
C      3.999536    −0.717969     2.677786
C      3.946168     2.479727    −2.921766
C      2.755624     1.504213     3.831865
C      3.764894    −4.036178    −0.311521
C      3.289554     0.188417     1.881946
C      3.821853    −1.627358    −0.395796
C      3.792693     1.301172    −0.824203
C      3.228483    −2.811160     0.063693
C      2.663197     1.301927     2.461021
C      3.430020     1.429128    −2.172693
H      3.306494    −4.955621     0.038175
H      3.667543     2.585071    −3.965451
H      2.272289     2.364706     4.283354
P      3.119175    −0.062335     0.119675
H      2.748497     0.717052    −2.628734
H      2.109881     2.004814     1.846327
H      2.352679    −2.776383     0.706396


LA−5f_N₂_LB−3
    74
xyz
C      3.664381    −1.485730    −1.975817
C      2.784132    −0.807704    −1.145292
C      1.390474    −0.922741    −1.197964
C      0.919837    −1.818109    −2.142758
C      1.769256    −2.516394    −3.005240
C      3.146672    −2.349842    −2.933159
S      3.447697     0.237284     0.136859
C      2.478426     1.696486    −0.162808
C      1.092575     1.519439    −0.251680
C      0.380725     2.694186    −0.422934
C      0.992952     3.946077    −0.521101
```

```
C     2.373423     4.068320    −0.439915
C     3.129562     2.918134    −0.250157
B     0.533030    −0.031916    −0.104684
C     1.124142    −0.560594     1.357735
C     0.501252    −1.173142     2.432265
C     1.185105    −1.565459     3.587943
C     2.553923    −1.377425     3.704414
C     3.231989    −0.802407     2.636716
C     2.514730    −0.419072     1.513354
F     4.979852    −1.328141    −1.867045
F     3.948579    −3.014100    −3.749864
F     1.261921    −3.352824    −3.895754
F    −0.385818    −2.089190    −2.264283
F     4.452042     3.004416    −0.151978
F     2.952434     5.253983    −0.531847
F     0.250787     5.028656    −0.689164
F    −0.957407     2.701026    −0.494512
F     4.549752    −0.636243     2.704990
F     3.199412    −1.751986     4.796880
F     0.518994    −2.132504     4.580976
F    −0.804987    −1.459974     2.427481
N    −0.968251    −0.061154    −0.481105
N    −1.812114    −0.000543     0.416868
H    −6.167556    −1.537239     0.260053
H    −6.023927    −0.225431    −1.771737
H    −6.365952     0.949302     0.387553
C    −5.789305     0.986323     1.315008
C    −5.363957     0.570597    −2.123823
C    −5.377367    −2.217743    −0.067312
H    −5.518326     0.664559    −3.204750
H    −5.617530    −3.208740     0.333385
H    −6.188166     1.814441     1.911186
H    −5.413055    −2.296509    −1.155020
H    −5.682868     1.512734    −1.673942
H    −5.976767     0.069796     1.876683
H    −4.074897    −1.820937    −2.587235
H    −4.806389    −1.439128     2.484190
H    −4.730518     2.822753    −0.414413
C    −3.869217     0.272119    −1.893327
C    −4.290006     1.252665     1.081544
C    −3.987423    −1.821416     0.465134
C    −3.462299    −0.934810    −2.759245
C    −3.992700    −1.979410     1.997927
C    −4.133606     2.664845     0.485228
H    −4.143372    −3.043192     2.212778
H    −3.608863    −0.646722    −3.806320
H    −4.494065     3.377260     1.235291
P    −3.533848    −0.055739    −0.054814
H    −4.032914     2.015498     3.066477
H    −3.288646     1.625283    −3.444774
H    −3.239718    −3.810928     0.185710
C    −3.027432     1.465079    −2.392452
C    −2.919074    −2.796149    −0.074579
C    −3.543543     1.266467     2.433820
```

```
H     −2.790744    −2.762105    −1.154730
H     −3.575487     0.317734     2.966207
H     −3.222932     2.397267    −1.866376
H     −3.092257     2.915623     0.276243
H     −3.044546    −1.688472     2.449709
H     −2.409311    −1.187473    −2.633438
H     −2.496934     1.553549     2.313932
H     −1.960475     1.246838    −2.338353
H     −1.947657    −2.628381     0.395166
```

LA−5f_N₂_LB−4
```
    67
xyz
C      2.294510    −2.133407    −2.401450
C      2.006863    −1.200211    −1.415815
C      0.807605    −1.142766    −0.695621
C     −0.087936    −2.156541    −0.993403
C      0.153027    −3.104403    −1.989511
C      1.340248    −3.094900    −2.709736
S      3.287518    −0.054762    −0.930645
C      2.346760     1.457108    −0.994155
C      1.134657     1.464057    −0.296388
C      0.484675     2.688076    −0.281595
C      0.979578     3.808424    −0.953036
C      2.176607     3.745505    −1.655469
C      2.879483     2.547458    −1.666539
B      0.697654     0.051346     0.444025
C      1.965019    −0.272190     1.444798
C      1.954781    −0.506057     2.809888
C      3.127417    −0.769993     3.524831
C      4.359316    −0.812132     2.882411
C      4.409667    −0.590015     1.511603
C      3.225524    −0.329928     0.837610
F      3.459421    −2.128577    −3.043017
F      1.565195    −3.999229    −3.651033
F     −0.758437    −4.034031    −2.247588
F     −1.233528    −2.315500    −0.313356
F      4.040941     2.466730    −2.309038
F      2.641795     4.811154    −2.289324
F      0.305746     4.948453    −0.919695
F     −0.658838     2.877421     0.395101
F      5.577671    −0.630969     0.875149
F      5.465702    −1.063799     3.566450
F      3.071612    −0.986162     4.829041
F      0.821628    −0.498762     3.515821
N     −0.633467     0.187484     1.179788
N     −1.630997     0.205577     0.463122
H     −3.742472     0.484833     3.067795
H     −6.008889    −0.063223    −1.654328
H     −2.177436     1.343929     2.959861
H     −6.003649     1.715252    −1.701951
C     −2.736509     0.457445     2.652770
N     −2.819460     0.419524     1.190003
C     −5.406641     0.815348    −1.898585
```

```
H     −5.170032      0.775705     −2.966269
H     −7.106322     −0.228465      2.341051
N     −4.156679      0.838135     −1.128743
H     −4.558288     −1.982093      2.064169
H     −2.202977     −0.424883      3.016711
H     −6.654476     −1.193128      0.921048
P     −4.192973      0.043603      0.312088
C     −6.738754     −0.179120      1.311117
H     −5.147323     −2.630578     −1.644733
C     −4.372487     −2.496908      1.118351
H     −3.842358      2.933019     −1.208913
C     −3.314475      1.996367     −1.429659
N     −5.441656      0.497066      1.294994
H     −5.880372      1.974472      2.725549
N     −4.380243     −1.553197     −0.003465
H     −3.404117     −3.005289      1.179580
H     −7.470134      0.369213      0.703737
C     −4.207020     −2.171558     −1.318561
C     −5.515353      1.906443      1.695815
H     −5.160347     −3.243948      0.975462
H     −3.065675      1.974747     −2.495260
H     −2.391114      1.960065     −0.859584
H     −3.890632     −1.430685     −2.052539
H     −3.435299     −2.943309     −1.258966
H     −4.532450      2.380776      1.649871
H     −6.201622      2.459702      1.042069
```

LA−5f_N₂_LB−5
```
   69
xyz
 C     −2.690127      1.618869     −0.218022
 C     −1.304938      1.469427     −0.362775
 C     −0.637540      2.636271     −0.699091
 C     −1.292267      3.858675     −0.870312
 C     −2.668018      3.956769     −0.711902
 C     −3.380198      2.811176     −0.379910
 B     −0.713190     −0.055213     −0.112775
 N      0.792325     −0.154926     −0.412844
 N      1.556757      0.350953      0.415426
 P      3.280539      0.102001      0.035046
 N      3.623415     −1.220834      0.974440
 C      2.969406     −2.510776      0.747743
 F      0.691070      2.669588     −0.886941
 F     −0.595617      4.938675     −1.188225
 F     −3.284918      5.116264     −0.875953
 F     −4.699041      2.874424     −0.224387
 S     −3.615525      0.157184      0.207999
 C     −2.629083     −0.388568      1.592457
 C     −1.245036     −0.494820      1.391940
 C     −0.548103     −0.999770      2.478727
 C     −1.172637     −1.333350      3.684182
 C     −2.544027     −1.188521      3.842197
 C     −3.287604     −0.714620      2.769031
 F      0.769399     −1.225629      2.437616
```

```
F    -0.449655   -1.802410    4.689748
F    -3.129918   -1.509137    4.985466
F    -4.606918   -0.587754    2.882689
C    -2.965628   -0.948526   -1.034132
C    -3.854648   -1.681607   -1.806401
C    -3.343228   -2.557350   -2.755980
C    -1.964425   -2.669721   -2.888072
C    -1.101716   -1.914624   -2.087765
C    -1.572247   -1.020214   -1.138461
F    -5.170566   -1.562757   -1.653036
F     0.204817   -2.117762   -2.287728
F    -1.467425   -3.508174   -3.784039
F    -4.152618   -3.277448   -3.517909
N     3.329231   -0.254487   -1.578507
C     4.294285   -1.235326   -2.056004
C     5.724002   -0.753373   -1.772433
N     5.762619   -0.239937   -0.410845
C     6.069461   -1.194644    0.646005
C     4.909196   -1.241897    1.662525
C     2.795258    0.676027   -2.571840
N     3.896692    1.528963    0.631906
C     5.325940    1.832031    0.790129
C     6.201147    1.131711   -0.234516
C     3.105642    2.416741    1.507341
H     2.048064    2.181654    1.460945
H     5.451038    2.914899    0.683626
H     3.257455    3.450143    1.181442
H     5.636888    1.581695    1.814819
H     5.982551    0.051129   -2.465751
H     3.607534    1.118490   -3.162275
H     3.445989    2.316578    2.545851
H     6.096025    1.644116   -1.193626
H     2.251646    1.486284   -2.087469
H     4.130045   -1.384549   -3.126529
H     6.446804   -1.562887   -1.930474
H     7.255627    1.205799    0.070133
H     2.103432    0.148418   -3.234643
H     4.116461   -2.199833   -1.572703
H     4.962852   -0.399848    2.358185
H     6.189533   -2.184265    0.194145
H     7.013442   -0.948857    1.150621
H     2.119960   -2.393136    0.071705
H     2.604655   -2.906580    1.699272
H     4.959819   -2.151394    2.267018
H     3.664466   -3.235744    0.305197
```

LA−5f_N₂_LB−6
```
    87
xyz
C    -3.587909   -2.399738    2.198879
C    -3.220724   -1.403411    1.305709
C    -1.917573   -0.926322    1.127318
C    -0.975295   -1.502767    1.968043
C    -1.299843   -2.520444    2.867947
```

```
C    −2.604547    −2.981291     2.987848
S    −4.498105    −0.616679     0.338877
C    −4.073900     1.088485     0.674232
C    −2.735385     1.456336     0.489665
C    −2.450031     2.783239     0.767255
C    −3.430563     3.682313     1.195638
C    −4.747691     3.272655     1.364333
C    −5.075744     1.949096     1.098956
B    −1.718432     0.260359    −0.016509
C    −2.433460    −0.311421    −1.396900
C    −1.925504    −0.367138    −2.686875
C    −2.659358    −0.882144    −3.758304
C    −3.956131    −1.347619    −3.578697
C    −4.516774    −1.278125    −2.310822
C    −3.750509    −0.767121    −1.272928
F    −4.851594    −2.800918     2.312338
F    −2.902881    −3.944326     3.848355
F    −0.351359    −3.056164     3.626092
F     0.307323    −1.112856     1.989362
F    −6.330534     1.533377     1.254874
F    −5.672299     4.130746     1.771390
F    −3.108279     4.942448     1.446220
F    −1.215266     3.281970     0.639685
F    −5.766164    −1.692646    −2.113592
F    −4.645622    −1.832454    −4.601439
F    −2.119427    −0.924291    −4.967821
F    −0.706837     0.093716    −2.996711
N    −0.263917     0.696753    −0.168769
N     0.462809    −0.237040    −0.570444
H     6.925923    −2.347178    −2.976092
H     8.593856    −2.747526    −1.183929
C     6.705031    −2.059122    −1.953024
C     7.642736    −2.282483    −0.943656
H     6.391337     1.802915    −0.409875
C     5.485613    −1.462562    −1.649222
C     7.364360    −1.909476     0.369862
H     7.576088     3.132107     1.337638
H     4.745995    −1.276762    −2.423642
C     5.890816     2.084733     0.511591
H     8.096564    −2.080282     1.152721
C     6.545565     2.827593     1.491067
C     5.212820    −1.108902    −0.329722
C     6.141739    −1.319430     0.682151
H     4.251345     3.071547    −1.586627
N     3.910417     0.905009    −0.290598
H     2.950587     4.110368    −3.303384
C     2.607976     1.201786    −0.682014
C     4.571356     1.702137     0.720472
N     3.956286    −0.489968     0.000358
H     5.900947    −1.025143     1.699112
C     3.300154     3.497748    −1.256949
C     1.836200     0.009280    −0.637492
C     2.673217     4.430468    −2.292900
C     2.734776    −1.031556    −0.307497
```

```
C      5.876047      3.183554      2.660509
H      3.006558      5.462253     -2.160952
H      0.993923      2.161916     -2.717851
N      2.299435      2.421690     -1.094623
H      4.255839     -3.548294     -0.052296
N      2.516952     -2.342874     -0.246816
H      1.147958     -2.687561     -1.822626
H      6.386160      3.768962      3.419238
H      3.461745      4.000186     -0.297872
C      1.042116      2.751387     -1.793411
C      3.895202      2.038904      1.891026
C      3.354903     -3.291019      0.514010
C      1.309171     -2.995442     -0.786600
H      2.210732     -4.853477     -1.454828
C      4.552214      2.790909      2.860009
C      1.171130      4.243726     -2.072796
H      3.658026     -2.840924      1.463637
C      1.616123     -4.481003     -0.612980
H      0.571266      4.548212     -2.933428
H      2.865713      1.720429      2.035686
H      0.193610      2.484600     -1.165370
C      2.442384     -4.505775      0.675512
H      0.430561     -2.694800     -0.209921
H      0.833733      4.817192     -1.202401
H      4.032166      3.068110      3.771661
H      0.703879     -5.078953     -0.550895
H      3.013525     -5.427505      0.806738
H      1.792130     -4.377947      1.548086
```

LA−8f_N$_2$_LB−1
```
    24
xyz
 C      1.481822     -0.295562      0.409562
 F      2.147556      0.437401      1.356234
 B     -0.142982     -0.022744      0.405524
 C     -0.921910     -1.141138     -0.513087
 F     -0.915476     -2.372846      0.081333
 C     -0.484560      1.506551     -0.079236
 F     -0.185417      1.750120     -1.374868
 F      1.811998     -1.593325      0.687187
 F      2.084277     -0.005810     -0.762067
 F     -1.794149      1.831598      0.073251
 F      0.201534      2.436546      0.648370
 F     -2.231152     -0.853333     -0.719608
 F     -0.375815     -1.316995     -1.736370
 N     -0.782757     -0.159548      1.816478
 N     -0.057147     -0.621906      2.673771
 N     -0.600163     -1.398408      6.154685
 H      1.819697     -1.919969      5.463213
 C     -0.022314     -1.178606      4.961199
 N     -0.738603     -0.735863      3.935591
 H     -1.582792     -1.217238      6.292371
 N      1.279412     -1.405055      4.785856
 H      1.659678     -1.262848      3.853825
```

```
H    −1.709467    −0.434158     3.984841
H    −0.039509    −1.540674     6.981006
```

LA−8f_N$_2$_LB−2
```
    49
xyz
C    −1.545283    −0.501426     0.856171
F    −1.173340    −1.408045     1.818732
B    −0.810326     0.952473     1.084007
C    −1.570556     2.152078     0.260848
F    −2.853004     2.349635     0.668199
C     0.786854     0.877903     0.708927
F     1.025592     0.784956    −0.620316
F    −2.897268    −0.447524     0.931961
F    −1.254789    −1.082461    −0.326019
F     1.483696     1.975056     1.129156
F     1.421202    −0.186555     1.275317
F    −0.954105     3.358064     0.443781
F    −1.628104     1.958255    −1.074574
N    −1.088412     1.272552     2.573090
N    −0.132457     1.256489     3.348096
H    −2.227286     3.577533     3.796298
H    −4.637764     4.064474     3.970282
C    −2.843515     3.010266     4.487633
C    −4.202144     3.284311     4.585944
H     2.078668     2.359564     4.144997
H     3.554277     4.251577     4.747221
C     1.753850     3.092844     4.877376
C     2.578900     4.160899     5.214478
P    −0.558240     1.602912     5.034896
C     0.489017     2.990952     5.472183
C     2.150809     5.113607     6.137769
C    −2.288126     1.986811     5.268507
H     2.799276     5.946121     6.394264
C     0.891584     5.009495     6.726922
C     0.054244     3.949448     6.394428
C    −5.001638     2.544251     5.455869
H    −6.064024     2.758433     5.525005
H     0.557466     5.757400     7.439308
H    −0.934328     3.875750     6.839691
H    −0.825115    −1.189519     4.367586
C    −3.092703     1.234089     6.130886
C    −4.449953     1.523234     6.227830
C    −0.089042     0.121473     5.930560
C    −0.372484    −1.122758     5.353358
H    −2.664568     0.427790     6.719632
C     0.522024     0.204786     7.185532
H     0.757624     1.172814     7.619841
H    −5.077492     0.945321     6.899015
C    −0.046460    −2.283990     6.046336
H    −0.254920    −3.250418     5.598705
C     0.840080    −0.963562     7.870839
C     0.554412    −2.203932     7.301819
H     1.317246    −0.905429     8.844182
```

| H | 0.810002 | −3.114045 | 7.836374 |

LA−8f_N₂_LB−3
```
    55
xyz
```

C	−2.844970	0.870394	1.118238
F	−2.485620	0.503330	2.379924
B	−2.069112	0.000287	−0.035598
C	−2.302688	0.643615	−1.529771
F	−1.598007	1.804342	−1.708352
C	−2.507378	−1.582289	0.010699
F	−3.740749	−1.820609	−0.478592
F	−2.537374	2.201743	1.040521
F	−4.191947	0.795025	1.078082
F	−1.655983	−2.373124	−0.713603
F	−2.486025	−2.109234	1.264888
F	−1.911462	−0.167455	−2.549935
F	−3.592802	0.959767	−1.784826
N	−0.579325	0.034296	0.388999
N	0.245106	−0.024446	−0.532861
H	1.099003	−0.240695	−2.805972
H	0.249616	−2.390666	1.024929
H	0.151205	2.308983	1.045477
H	1.447994	−2.682770	−1.150296
H	0.553259	0.492170	2.691773
H	1.464887	2.162548	−1.952675
C	1.185097	−2.240616	1.565677
C	2.183516	−0.354777	−2.752232
C	1.214095	2.556102	1.042137
P	1.919515	0.010618	0.028699
H	1.455369	3.032898	0.094006
H	0.980988	−1.598914	2.419672
H	2.423472	−1.416034	−2.718278
H	1.503435	−3.216265	1.951645
H	1.380956	3.297589	1.832032
H	2.616128	0.042810	−3.677493
C	2.360012	−2.716197	−0.547963
C	1.597028	0.809736	2.740083
C	2.534735	1.936288	−1.909240
C	2.309610	−1.733861	0.637365
C	2.794516	0.452081	−1.581878
C	2.095307	1.331736	1.377272
H	1.658313	1.645540	3.446724
H	2.438319	−3.726683	−0.131242
H	2.949980	2.133672	−2.903707
H	2.211933	0.003754	3.145453
H	3.025375	2.622532	−1.216470
H	3.229820	−2.564943	−1.190807
C	3.565457	1.768882	1.515978
C	4.308826	0.195179	−1.516803
C	3.661455	−1.765730	1.373566
H	3.639923	−1.214979	2.316399
H	4.545411	−0.867934	−1.423252
H	3.931206	2.304998	0.637225

```
H      3.891323     −2.810188      1.614170
H      3.632372      2.458968      2.364932
H      4.754086      0.542017     −2.456436
H      4.241534      0.933853      1.721307
H      4.486189     −1.381801      0.766342
H      4.802294      0.732564     −0.702653
```

LA−8f_N$_2$_LB−4
```
   48
xyz
 C      0.623666      0.224425      0.913423
 F      1.483430      0.127703      1.977189
 B     −0.755168      1.040595      1.282284
 C     −1.871781      0.831676      0.093067
 F     −2.423046     −0.418952      0.114911
 C     −0.437063      2.637007      1.506575
 F     −0.176106      3.320714      0.374769
 F      0.383801     −1.071538      0.553037
 F      1.350775      0.760659     −0.089120
 F     −1.470068      3.293654      2.112855
 F      0.636814      2.860074      2.329989
 F     −2.924146      1.688716      0.168827
 F     −1.364521      0.982717     −1.155110
 N     −1.223956      0.459954      2.637810
 N     −2.431395      0.492455      2.859189
 H     −4.448582      0.344423      5.335693
 H     −2.235001      2.181654      5.779879
 H     −4.567132     −1.153770      4.367983
 H     −0.645203      2.847800      6.197167
 C     −4.195477     −0.124448      4.380199
 N     −2.763212     −0.059432      4.116230
 C     −1.183899      2.217178      5.482095
 H     −1.119592      2.665045      4.485153
 H     −0.188162     −3.493404      5.943504
 N     −0.588612      0.876530      5.490701
 H     −3.329763      0.730607      7.817228
 H     −4.677299      0.432198      3.574234
 H      0.044601     −1.942850      6.780022
 P     −1.565625     −0.419777      5.234140
 C      0.102513     −2.444538      5.811588
 H     −4.214024     −1.648480      6.938852
 C     −2.377550      0.182451      7.796379
 H      1.417636      1.333680      5.873643
 C      0.819616      0.864620      5.084900
 N     −0.789274     −1.808826      4.843787
 H     −0.722889     −3.447912      3.567477
 N     −2.313757     −0.747252      6.677334
 H     −1.551960      0.892527      7.748708
 H      1.140442     −2.411929      5.458893
 C     −3.159052     −1.927366      6.821171
 C     −0.701125     −2.355733      3.487125
 H     −2.285625     −0.384029      8.729651
 H      0.949091      1.405382      4.144783
 H      1.171605     −0.155358      4.934245
```

```
H   -3.063477   -2.575195    5.947114
H   -2.846733   -2.496024    7.705329
H   -1.548741   -2.037138    2.882409
H    0.219677   -2.041684    2.988645
```

LA-8f_N₂_LB-5
```
    50
xyz
C    3.630846    6.509815    3.299725
F    3.423631    7.579611    2.480468
B    2.328576    6.144862    4.231758
C    2.683858    4.963176    5.318104
F    3.573273    5.402463    6.263154
C    1.026009    5.748926    3.312536
F    1.186558    4.640525    2.559150
F    4.737726    6.830221    4.032163
F    4.014778    5.498133    2.483756
F   -0.104103    5.544714    4.045475
F    0.697035    6.752468    2.442414
F    1.603614    4.540325    6.029056
F    3.234337    3.854644    4.780451
N    1.833372    7.312576    5.110832
N    2.472919    8.373253    5.070779
H    1.401649    6.842735    7.976967
H   -0.975250    9.174072    7.095430
H    1.891107    8.096849    9.166457
C    1.850328    7.832078    8.103069
H   -0.515363    8.497567    8.649885
H   -1.201226   11.953664    6.622148
C   -0.221365    9.224849    7.887888
H   -1.501444    9.728865    4.880870
H    2.874168    7.782390    7.727885
H   -1.170771   11.032007    8.649466
H   -0.357567    8.374542    4.755381
C   -0.515965    9.425471    4.504959
H   -0.413134   11.949118    4.353010
N    0.536753   10.259328    5.093458
N    1.081082    8.838712    7.369762
C   -0.135893   12.180476    6.508658
C   -0.158806   10.646196    8.469449
C    0.332294   11.700780    5.114023
H   -0.024945   13.272400    6.586365
P    1.712601    9.612291    6.061473
N    0.587688   11.497315    7.562092
H    0.352041   10.621036    9.436408
H   -0.498946    9.518453    3.415240
H    1.257023   12.206539    4.820229
C    1.842209   12.045617    8.026510
N    2.995749   10.652278    6.282235
C    2.928778   11.947748    6.965418
H    3.899725   12.124334    7.443102
H    1.755433   13.099528    8.339662
H    2.154370   11.466904    8.899257
C    4.111417   10.653184    5.312596
```

```
H    4.201405     9.693037     4.812141
H    5.036912    10.859852     5.858731
H    2.805365    12.743527     6.214632
H    3.960794    11.439185     4.559920

LA−8f_N₂_LB−6
    68
xyz
C   −4.071567     0.515442    −1.566149
F   −3.637033     1.774810    −1.877852
B   −3.394986    −0.053972    −0.181562
C   −3.725058    −1.654352     0.005493
F   −2.980228    −2.440781    −0.837779
C   −3.940444     0.803281     1.114034
F   −5.216862     0.526788     1.466079
F   −3.752926    −0.243047    −2.654314
F   −5.424119     0.594585    −1.554239
F   −3.193652     0.598170     2.237886
F   −3.897789     2.157298     0.917981
F   −3.461767    −2.140510     1.252474
F   −5.013584    −1.986634    −0.245591
N   −1.882822     0.223163    −0.328196
N   −1.138264    −0.434384     0.423596
H    4.089061     3.175949     3.275983
C    4.165458     2.841375     2.245864
H    6.015157     3.880803     1.878297
H    1.387828    −4.051934     3.056372
C    5.248654     3.236097     1.458750
H    2.331728     1.700069     2.311938
C    3.181029     2.016730     1.712058
C    1.510138    −4.381166     2.018199
H    2.089847    −5.307712     2.018709
H    2.929918    −2.710703     1.759390
C    5.348207     2.806276     0.137305
C    2.190174    −3.287491     1.195879
H   −0.741123    −2.589937     1.884932
H   −0.603435    −5.004688     1.966839
C    0.144679    −4.514493     1.340160
C    3.283003     1.605421     0.384878
H    5.014615    −1.077904     0.643899
C   −0.241168    −3.068702     1.039155
H   −0.972037     2.482262     1.342747
N    1.069514    −2.418361     0.796950
H    6.191206     3.112409    −0.474640
C    1.210775    −1.137649     0.473296
C    4.359273     1.988263    −0.405773
N    2.462667    −0.614795     0.184533
C    0.234972    −0.138060     0.304855
H   −0.233279     4.780464     0.953861
H    2.682566    −3.707292     0.311413
C    4.689689    −1.467355    −0.316155
C    0.921862     1.041329    −0.052561
N    2.275824     0.747941    −0.187999
C   −0.809191     2.783983     0.304994
```

```
N      0.502418     2.298328    −0.166741
H      2.037903     3.765482    −0.262715
H      0.236298    −5.087295     0.410011
C      3.363306    −1.313852    −0.700243
C     −0.717737     4.292831     0.099154
H      6.612876    −2.248977    −0.876575
H     −0.889731    −2.958693     0.170984
C      1.239261     3.351876    −0.888312
C      5.574929    −2.123083    −1.169280
H      4.408697     1.649946    −1.436231
H     −1.709177     4.731150    −0.031575
H     −1.598069     2.341564    −0.306869
C      0.162938     4.404768    −1.148147
H      1.688486     2.938127    −1.796244
H      0.595630     5.398368    −1.290258
C      2.905764    −1.794753    −1.925088
C      5.125549    −2.621085    −2.390602
H      1.865570    −1.654688    −2.207962
C      3.792011    −2.457252    −2.768084
H     −0.415479     4.145265    −2.041303
H      5.814679    −3.138384    −3.051423
H      3.442452    −2.843428    −3.720651
```

LA−4_N₂_LA−4
```
   10
xyz
 N     −1.336997     1.514523    −0.351714
 N     −0.167120     1.799034    −1.204415
 N      0.020839     1.299556     0.168759
 B     −0.517452     0.395316    −0.879019
 N     −0.543540    −0.913542    −1.342325
 N     −0.565307    −1.979637    −1.720471
 N     −0.267858    −4.700602    −1.866377
 N     −0.097742    −4.206657    −3.241967
 B     −0.590903    −3.288140    −2.184472
 N     −1.450430    −4.386001    −2.690659
```

LA−5a_N₂_LA−5a
```
   68
xyz
 C     −2.165224     1.599087     2.299890
 C     −2.728750     0.875197     1.257502
 C     −4.126614     0.775457     1.152920
 C     −4.945560     1.397351     2.084323
 C     −4.373100     2.126080     3.131284
 C     −2.989939     2.226593     3.239528
 B     −2.082132     0.050017     0.035310
 C     −2.608784    −1.471346     0.136360
 C     −4.013098    −1.443725     0.094204
 C     −4.738794    −2.624164     0.163918
 C     −4.065723    −3.844629     0.275775
 C     −2.675724    −3.876220     0.315540
 C     −1.944674    −2.685605     0.245146
 C     −4.626865    −0.049709    −0.032560
```

```
C    −4.054504     0.583247    −1.300520
C    −2.652573     0.673700    −1.337098
C    −2.025673     1.233207    −2.442360
C    −2.791113     1.703150    −3.514810
C    −4.178408     1.610848    −3.475004
C    −4.814435     1.049195    −2.363652
H    −5.899433     0.977883    −2.332732
H    −4.771409     1.976358    −4.308602
H    −2.298766     2.141233    −4.378497
H    −0.940299     1.316645    −2.490361
H    −5.825809    −2.600176     0.131164
H    −4.632010    −4.770092     0.330521
H    −2.154399    −4.825581     0.400208
H    −0.856252    −2.731035     0.274453
H    −6.027216     1.318207     2.000656
H    −5.012162     2.613892     3.861912
H    −2.547081     2.792102     4.054629
H    −1.084007     1.686740     2.401835
H    −5.719454    −0.091891    −0.061448
N    −0.552456     0.088573     0.063906
N     0.552481     0.085118     0.066198
H     2.525654     4.839753     0.892291
H     4.991512     4.603697     0.799397
C     2.972803     3.866897     0.707994
C     4.356435     3.734158     0.655433
C     2.153135     2.748607     0.522919
H     1.071420     2.872017     0.565312
C     4.934475     2.483647     0.416546
H     6.016529     2.380535     0.374443
C     2.722209     1.504252     0.286753
H     2.144217    −1.617344    −4.560132
C     2.667522    −1.302472    −3.661674
C     4.120554     1.375145     0.233107
C     4.057803    −1.318364    −3.622143
H     4.622291    −1.645022    −4.490934
C     1.938716    −0.882478    −2.543881
H     0.850101    −0.880259    −2.592964
C     4.733443    −0.916492    −2.465839
C     2.605377    −0.480269    −1.394439
C     4.010000    −0.499975    −1.357692
H     5.820682    −0.930841    −2.434918
B     2.081957     0.047944     0.037330
C     4.626961    −0.041521    −0.036708
H     5.719643    −0.079448    −0.068031
C     2.662346    −0.945926     1.165554
C     4.063868    −0.942592     1.062170
C     2.043315    −1.729101     2.130469
C     4.831271    −1.718645     1.918713
H     0.958387    −1.744207     2.230646
H     5.915927    −1.714235     1.836470
C     2.816260    −2.512033     2.994474
C     4.203140    −2.506494     2.888137
H     2.330195    −3.123877     3.749223
H     4.801971    −3.115043     3.559849
```

LA−5d_N₂_LA−5d

    66

xyz
```
  C      4.629764       0.082268      -2.829086
  C      3.964370       0.046966      -1.612510
  C      2.570793       0.044179      -1.486669
  C      1.827205       0.078976      -2.661525
  C      2.468285       0.115090      -3.903797
  C      3.856986       0.116879      -3.990587
  S      4.896035       0.001030      -0.070225
  C      4.075504       1.349269       0.800061
  C      2.677814       1.295563       0.832165
  C      2.018662       2.324522       1.496659
  C      2.744425       3.356599       2.099396
  C      4.134820       3.376630       2.047330
  C      4.824178       2.358493       1.387538
  B      2.111767      -0.000732       0.060030
  C      2.675844      -1.340670       0.755049
  C      2.015077      -2.405477       1.358725
  C      2.739152      -3.472119       1.900180
  C      4.129527      -3.491408       1.846565
  C      4.820504      -2.437663       1.247079
  C      4.073435      -1.394640       0.719566
  H      5.714276       0.083185      -2.882829
  H      4.344640       0.145068      -4.959125
  H      1.873903       0.142037      -4.811661
  H      0.738556       0.078696      -2.636568
  H      5.908943       2.362142       1.339593
  H      4.688381       4.181770       2.518409
  H      2.215456       4.152054       2.614769
  H      0.932046       2.343981       1.560030
  H      5.905252      -2.440303       1.198699
  H      4.681830      -4.323541       2.269867
  H      2.208902      -4.295251       2.368646
  H      0.928437      -2.426709       1.421314
  N      0.550739      -0.001115       0.111460
  N     -0.551028      -0.000533       0.111301
  H     -4.462442       4.301641      -2.421469
  H     -1.990884       4.271446      -2.292921
  C     -3.952234       3.473321      -1.941717
  C     -2.562916       3.452876      -1.867578
  C     -4.696583       2.425864      -1.397564
  H     -5.781207       2.429587      -1.448787
  C     -1.892952       2.391348      -1.251395
  H     -0.805015       2.413011      -1.213074
  C     -4.002741       1.387805      -0.793325
  C     -2.607790       1.333540      -0.699545
  C     -3.945931      -3.390739      -2.085085
  C     -4.692173      -2.368276      -1.497698
  C     -2.556641      -3.371009      -2.010025
  H     -4.454618      -4.199175      -2.599143
  C     -4.000237      -1.355177      -0.850427
  H     -5.776786      -2.371691      -1.549173
```

```
S    -4.896090    -0.000150    -0.069343
C    -1.888597    -2.334980    -1.349979
H    -1.983143    -4.170065    -2.469147
C    -2.605357    -1.302486    -0.754387
B    -2.112121    -0.000366     0.060071
H    -0.800618    -2.356262    -1.312722
C    -4.110847    -0.033053     1.552581
C    -2.711804    -0.032033     1.554502
C    -4.885731    -0.057449     2.702946
H    -5.970584    -0.057190     2.657061
C    -2.079182    -0.057561     2.793109
H    -0.993098    -0.058489     2.866461
C    -4.222579    -0.082558     3.930471
C    -2.831616    -0.082623     3.971371
H    -4.796892    -0.102144     4.850461
H    -2.323259    -0.102431     4.930209

LA-5e_N₂_LA-5e
   68
xyz
C     4.847981    -0.555478    -2.543444
C     4.111541    -0.305321    -1.397698
C     2.708092    -0.320427    -1.456421
C     2.078480    -0.583403    -2.650041
C     2.807865    -0.836492    -3.808890
C     4.192361    -0.821158    -3.749511
C     4.680292     0.001350    -0.002293
F     6.041144     0.002693    -0.004803
B     2.116215    -0.001409     0.002568
C     2.709769     1.421492     0.453664
C     4.113147     1.363132     0.431936
C     4.850900     2.480491     0.785371
C     4.196665     3.657733     1.161029
C     2.812243     3.716654     1.183012
C     2.081507     2.586522     0.825491
F     6.181856     2.498193     0.787959
F     4.907491     4.728405     1.499652
F     2.195986     4.838242     1.540952
F     0.736615     2.659117     0.851817
F     0.733489    -0.601897    -2.723464
F     2.190281    -1.089712    -4.957941
F     4.901939    -1.060904    -4.847373
F     6.178909    -0.557536    -2.562589
C     2.713487    -1.103460     1.007058
C     2.088151    -2.007644     1.832659
C     2.821750    -2.882454     2.629872
C     4.206025    -2.834357     2.584363
C     4.857279    -1.920625     1.750109
C     4.116709    -1.055682     0.962040
F     0.743457    -2.065997     1.887671
F     6.188266    -1.932109     1.758978
F     4.919589    -3.663078     3.339568
F     2.208360    -3.752943     3.424763
N     0.547941    -0.002760     0.004574
```

77

```
N    −0.547952    −0.002735     0.004378
F    −2.188514     3.750532    −3.420170
F    −4.900227     3.665951    −3.344828
C    −2.806504     2.881197    −2.627576
C    −4.191019     2.835811    −2.587098
F    −0.732476     2.061028    −1.877940
C    −2.077479     2.004941    −1.827767
C    −4.847007     1.923337    −1.755205
F    −6.177926     1.937386    −1.768755
C    −2.707478     1.101845    −1.004491
C    −4.110952     1.056935    −0.964529
B    −2.116185    −0.001576     0.002309
F    −0.739255    −2.665551    −0.840226
C    −2.711166    −1.423236    −0.450744
C    −2.084069    −2.589832    −0.819611
C    −4.680245     0.001237    −0.002169
C    −4.114480    −1.361795    −0.434251
C    −2.815946    −3.718441    −1.179608
F    −2.200830    −4.841554    −1.534710
C    −4.200314    −3.656401    −1.163035
C    −4.853361    −2.477608    −0.790191
F    −6.041101     0.002833    −0.004540
F    −4.912220    −4.725594    −1.504057
F    −6.184335    −2.492357    −0.797769
C    −2.712615     0.318758     1.458989
C    −4.115851     0.306830     1.395244
C    −2.086560     0.580102     2.654811
F    −0.741803     0.595025     2.732831
C    −4.855762     0.558742     2.538351
F    −6.186745     0.563913     2.552760
C    −2.819455     0.834944     3.811069
C    −4.203775     0.822935     3.746731
F    −2.205400     1.086658     4.962337
F    −4.916693     1.064406     4.842053


LA−5f_N₂_LA−5f
     66
xyz
   C     4.853189     0.245294    −2.729029
   C     4.131629     0.138707    −1.549745
   C     2.730272     0.131171    −1.513719
   C     2.075966     0.234742    −2.720052
   C     2.768879     0.344103    −3.930075
   C     4.159960     0.349915    −3.937595
   S     4.985300     0.001808     0.019391
   C     4.100426     1.281588     0.908055
   C     2.699889     1.236358     0.861565
   C     2.022795     2.221840     1.543391
   C     2.692378     3.224462     2.252241
   C     4.082932     3.245646     2.282743
   C     4.798989     2.259107     1.600165
   B     2.155959    −0.002509    −0.014327
   C     2.706504    −1.373206     0.629444
   C     2.034681    −2.465707     1.128539
```

```
C      2.709551    -3.573485     1.651460
C      4.100171    -3.592814     1.678149
C      4.810936    -2.498492     1.179008
C      4.107093    -1.418533     0.668342
F      6.173802     0.249104    -2.726431
F      4.817490     0.451793    -5.071208
F      2.104704     0.440873    -5.060551
F      0.734188     0.232141    -2.759220
F      6.119335     2.271338     1.622877
F      4.718624     4.185446     2.946433
F      2.006369     4.147813     2.889076
F      0.680445     2.241585     1.541003
F      6.131333    -2.507703     1.200009
F      4.740751    -4.630562     2.168611
F      2.028424    -4.596577     2.118357
F      0.692494    -2.490505     1.122936
N      0.547515    -0.004648    -0.031525
N     -0.547009    -0.003947    -0.032100
F     -1.985689    -0.444187     5.029103
F     -4.697544    -0.443829     5.104099
C     -2.676223    -0.344808     3.914626
C     -4.066585    -0.344872     3.955213
F     -0.668817    -0.242859     2.698128
C     -2.011418    -0.238734     2.688640
C     -4.787392    -0.237996     2.763284
F     -6.107671    -0.236619     2.791722
C     -2.693228    -0.132467     1.497531
C     -4.093521    -0.134894     1.567241
F     -0.711356     2.476349    -1.194690
C     -2.053285     2.458587    -1.166245
B     -2.155681    -0.001376    -0.016813
C     -2.736354     3.568603    -1.673609
F     -2.063094     4.588434    -2.158616
C     -2.717297     1.370054    -0.648521
C     -4.127172     3.593831    -1.665104
C     -4.118168     1.421069    -0.652216
C     -4.830014     2.503309    -1.146799
F     -4.775385     4.633871    -2.140439
S     -4.985064     0.004217     0.019455
F     -6.150463     2.518223    -1.134862
C     -2.725555    -1.238707    -0.877394
C     -4.126907    -1.279430    -0.889205
C     -2.068601    -2.226012    -1.575823
F     -0.726833    -2.248054    -1.607713
C     -4.845540    -2.255081    -1.563163
F     -6.166072    -2.262960    -1.553306
C     -2.758745    -3.227256    -2.266861
C     -4.149674    -3.244417    -2.262298
F     -2.091809    -4.152963    -2.920176
F     -4.804571    -4.183003    -2.908873
```

LA−1_N$_2$_LA−1
    20
xyz
```

```
N     −3.208661     −0.199195     −0.164340
H     −4.144856      0.112166     −0.434127
H     −2.792809     −0.876775     −0.793305
N     −1.028079      0.671718      0.193279
H     −0.472848      1.515474      0.118872
H     −0.764411      0.145030      1.021038
N     −2.978849      2.052329      0.223222
H     −2.429477      2.894781      0.410270
C     −2.403563      0.886524      0.077026
N     −5.799333      5.815729     −1.061935
H     −5.097851      5.285119     −1.584046
C     −6.206237      5.101316      0.037777
H     −7.221249      6.426015      1.196259
N     −5.478395      4.077816      0.404125
H     −5.730487      3.512810      1.218851
N     −7.344614      5.537189      0.720008
H     −6.568607      6.162679     −1.623651
H     −7.734052      4.848024      1.351717
N     −4.311153      2.250291      0.015807
N     −4.425110      3.619640     −0.329197
```

LA−2_N$_2$_LA−2
```
   70
xyz
P      1.944620      0.031669      0.172886
C      2.273130      0.586860     −1.549195
C      1.675194     −0.162963     −2.566516
C      3.085606      1.673067     −1.884928
C      1.887781      0.165378     −3.901730
H      1.028841     −0.996078     −2.300195
C      3.298693      2.002924     −3.222779
H      3.550475      2.268102     −1.103279
C      2.701010      1.249464     −4.231247
H      1.415316     −0.422567     −4.683930
H      3.929085      2.850803     −3.476256
H      2.866723      1.508645     −5.273505
C      2.490305      1.448262      1.190551
C      3.559818      1.349807      2.085096
C      1.759205      2.642564      1.120117
C      3.903723      2.433438      2.891691
H      4.128795      0.426781      2.157187
C      2.103224      3.720444      1.930443
H      0.913393      2.712663      0.442582
C      3.176985      3.619110      2.814696
H      4.739559      2.348811      3.580634
H      1.530107      4.641803      1.872644
H      3.444887      4.463006      3.444680
C      3.083568     −1.343596      0.472514
C      2.713847     −2.334799      1.387927
C      4.326149     −1.414250     −0.163081
C      3.582398     −3.388510      1.658309
H      1.741218     −2.269192      1.866624
C      5.195331     −2.466550      0.116344
H      4.615758     −0.652749     −0.882713
```

```
C    4.824145   −3.453906    1.026822
H    3.290079   −4.159308    2.365927
H    6.159413   −2.517069   −0.381671
H    5.501464   −4.275758    1.242440
H   −2.866853   −1.548371   −5.261996
C   −2.701177   −1.281183   −4.221756
H   −3.931982   −2.874641   −3.454622
H   −1.412729    0.385228   −4.687147
C   −3.300405   −2.025740   −3.207599
C   −1.886435   −0.195758   −3.900510
C   −3.087285   −1.685652   −1.872333
C   −1.673895    0.142866   −2.567850
C   −2.273320   −0.598019   −1.544889
H   −3.553207   −2.273818   −1.086116
H   −1.026449    0.977129   −2.307871
H   −0.914029   −2.709211    0.460304
H   −1.529811   −4.628195    1.904367
C   −1.759175   −2.634192    1.138154
C   −2.102647   −3.706312    1.956311
P   −1.944836   −0.029941    0.172975
C   −2.489921   −1.439264    1.200984
C   −3.175495   −3.598543    2.840911
H   −4.616603    0.645933   −0.886806
H   −3.442988   −4.437978    3.476999
C   −3.558479   −1.334277    2.095925
C   −3.901845   −2.412166    2.910400
C   −4.326923    1.412822   −0.172943
C   −3.084102    1.347177    0.462697
H   −4.127160   −0.410623    2.162120
H   −4.736955   −2.322528    3.599590
C   −5.196238    2.466974    0.098991
H   −6.160515    2.513582   −0.399029
C   −2.714256    2.345233    1.370593
H   −1.741428    2.283337    1.849389
C   −4.824930    3.461151    1.001964
C   −3.582932    3.400728    1.633461
H   −5.502357    4.284430    1.211718
H   −3.290532    4.176841    2.335215
N    0.492052   −0.534856    0.476311
N   −0.492365    0.539073    0.472193
```

LA−3_N₂_LA−3
```
  82
xyz
 P    2.015843    0.009994    0.001459
 C    2.570038   −0.653468   −1.717853
 C    2.985047    1.587318    0.416462
 C    2.376945   −1.362776    1.291448
 C    2.607749    0.516785   −2.718404
 H    3.451741    1.191555   −2.557232
 H    2.715516    0.107566   −3.731101
 H    1.682010    1.098959   −2.692633
 C    1.463172   −1.600024   −2.232072
 H    1.647017   −1.809258   −3.294709
```

```
H    1.436989    −2.556962    −1.711282
H    0.476652    −1.143697    −2.123357
C    3.926603    −1.373527    −1.768935
H    4.140174    −1.650529    −2.810525
H    4.753139    −0.746293    −1.422756
H    3.935113    −2.297239    −1.185912
C    2.376134     2.778836    −0.352186
H    2.846785     3.701457     0.012445
H    2.545690     2.729278    −1.427643
H    1.300036     2.835784    −0.178478
C    2.818051     1.924149     1.911315
H    3.321455     1.213041     2.570080
H    3.269089     2.907188     2.097010
H    1.761252     1.979538     2.185975
C    4.488811     1.502790     0.105730
H    4.693142     1.421674    −0.964262
H    4.968140     2.426574     0.454132
H    4.982313     0.668664     0.610961
C    3.849876    −1.489718     1.712962
H    3.946031    −2.347239     2.392643
H    4.520925    −1.667786     0.867962
H    4.209891    −0.611375     2.255211
C    1.508000    −1.062760     2.529014
H    1.662850    −1.863658     3.264797
H    1.750170    −0.118673     3.017189
H    0.452926    −1.043597     2.245104
C    1.896958    −2.735819     0.781142
H    0.863395    −2.680969     0.431094
H    2.527483    −3.144586    −0.011371
H    1.937368    −3.445037     1.618836
H   −1.937852     3.444064     1.621053
H   −0.864153     2.681098     0.432350
C   −1.897586     2.735457     0.782835
H   −1.440166     2.559613    −1.711673
H   −2.528532     3.144666    −0.009139
H   −1.663311     1.861164     3.266236
C   −1.463282     1.601778    −2.230999
H   −0.452740     1.043313     2.245560
H   −0.476189     1.147392    −2.119244
H   −1.645047     1.809126    −3.294354
C   −1.507821     1.061202     2.529557
C   −2.377057     1.361925     1.292315
H   −3.946152     2.344796     2.394935
H   −3.935879     2.297422    −1.185974
C   −3.849968     1.488134     1.714178
C   −2.569864     0.654358    −1.717716
C   −3.926685     1.373863    −1.769161
P   −2.015750    −0.009893     0.001333
H   −1.749183     0.116340     3.016737
H   −4.521141     1.667164     0.869498
H   −4.139842     1.651093    −2.810774
H   −4.209964     0.609042     2.255240
C   −2.606737    −0.515569    −2.718667
H   −2.715193    −0.106137    −3.731206
```

```
H     −1.680461     −1.096897     −2.693275
H     −4.753183      0.746289     −1.423591
H     −1.760534     −1.980414      2.184170
C     −2.985094     −1.587265      0.415488
H     −3.320918     −1.215002      2.569608
C     −2.817457     −1.925243      1.909988
H     −3.450030     −1.191194     −2.557493
H     −1.301258     −2.837747     −0.178895
H     −4.981445     −0.666583      0.609808
C     −2.376981     −2.778591     −0.354103
C     −4.489003     −1.501927      0.105515
H     −2.544737     −2.727170     −1.429742
H     −4.693954     −1.422181     −0.964477
H     −3.267986     −2.908656      2.094970
H     −2.849697     −3.700962      0.008514
H     −4.968935     −2.424771      0.455563
N     −0.505154     −0.524166      0.044415
N      0.505256      0.524135      0.044787
```

LA−4_N$_2$_LA−4
```
    68
xyz
P      2.342055     −0.032118     −0.089705
N      4.093165      0.237657     −0.216192
N      2.518366     −1.302866      1.037552
N      1.934063      1.430259      0.694491
C      4.859010     −0.867501     −0.778037
H      4.862436     −0.859341     −1.881046
H      4.454726     −1.831056     −0.457234
H      5.904310     −0.809034     −0.442767
C      4.489359      1.476052     −0.863947
H      4.041260      2.340032     −0.371597
H      4.208090      1.510172     −1.931945
H      5.580055      1.584947     −0.796983
C      3.623951     −1.450297      1.973034
H      4.315306     −0.613296      1.897099
H      4.182351     −2.380294      1.780294
H      3.233396     −1.509447      3.000468
C      1.645001     −2.463271      1.096153
H      0.825474     −2.349062      0.389443
H      1.245935     −2.594763      2.114227
H      2.213173     −3.373505      0.844290
C      1.388824      2.549425     −0.054673
H      0.952299      2.200177     −0.990070
H      2.158710      3.309756     −0.272584
H      0.593604      3.035458      0.528675
C      2.608377      1.816311      1.915092
H      2.782874      0.948482      2.554192
H      1.958503      2.507721      2.468603
H      3.575343      2.321962      1.747705
N      1.882551     −0.064266     −1.715514
C      2.166424     −0.977292     −2.801740
H      3.041244     −0.627254     −3.361110
H      1.307059     −0.974569     −3.484453
```

```
H      2.344534     −2.011370     −2.466063
H     −2.279487      3.207275     −0.694321
H     −3.132153      2.634402     −2.153472
C     −2.532625      2.318283     −1.290009
H     −4.340550      2.809840      0.671398
H     −5.215389      2.200661     −0.750834
H     −1.597982      1.852819     −1.619037
C     −4.538520      1.913882      0.064740
H     −0.709202      1.730029      1.724461
N     −3.307095      1.372716     −0.488374
H     −0.067066     −0.527850      1.818460
C     −1.711938      1.457776      2.077993
H     −5.037538      1.170574      0.689542
C     −1.079270     −0.859568      2.077088
H     −2.431678      2.199439      1.729699
N     −2.062267      0.117798      1.606841
H     −1.730417      1.453848      3.173721
P     −2.631773     −0.046002      0.050322
H     −1.953800     −0.624344     −2.989226
H     −1.172957     −0.960084      3.165250
H     −1.245745     −1.834756      1.616858
N     −1.472895     −0.625960     −0.921350
C     −1.702190     −1.322905     −2.178072
H     −4.674469     −0.429053     −1.748438
H     −0.765861     −1.829683     −2.427714
N     −3.971474     −1.047813      0.134384
C     −4.850250     −1.218062     −1.014077
H     −2.487102     −2.080255     −2.076376
H     −5.897207     −1.161166     −0.688004
C     −4.051554     −2.123243      1.109564
H     −3.601480     −1.810626      2.053201
H     −4.695763     −2.189992     −1.503473
H     −5.107711     −2.347995      1.298142
H     −3.560232     −3.043153      0.758509
N      0.793422     −0.500056     −0.758976
N     −0.353369      0.300907     −0.847919
```

LA−5_N₂_LA−5
      72
xyz
```
P     −1.916888     −0.203670     −0.271557
N     −5.092905      0.283460      0.428114
N     −2.605001      1.043269     −1.156072
N     −2.863839     −1.567412     −0.464046
N     −2.181479      0.251533      1.338693
C     −4.991377      1.426006     −0.448941
H     −5.632445      2.244994     −0.079723
H     −5.390164      1.135512     −1.428540
C     −3.570813      1.986100     −0.619658
H     −3.608450      2.852285     −1.292817
H     −3.221599      2.363555      0.347540
C     −4.662301      0.411710      1.800067
H     −5.411513     −0.036392      2.475117
H     −4.630028      1.481385      2.041165
```

```
C    −3.301578    −0.230349     2.126836
H    −3.071511    −0.050923     3.186380
H    −3.391271    −1.316328     2.011528
C    −5.293454    −1.028630    −0.139294
H    −6.243495    −1.057965    −0.699598
H    −5.399368    −1.739697     0.689562
C    −4.174952    −1.506273    −1.082364
H    −4.422640    −2.508208    −1.458210
H    −4.140188    −0.847338    −1.957095
C    −2.261476     1.188296    −2.561932
H    −1.497612     0.452421    −2.820193
C    −1.358017     1.293255     1.929386
H    −0.585838     1.589873     1.214560
C    −2.436868    −2.856951     0.044424
H    −1.486158    −2.751111     0.569643
H    −1.951551     2.181263     2.200383
H    −0.858878     0.927645     2.838034
H    −1.847919     2.186240    −2.753505
H    −3.139711     1.038490    −3.209349
H    −2.287670    −3.572494    −0.775442
H    −3.177985    −3.276767     0.742508
H     3.138975    −1.030680    −3.211513
H     4.422806     2.510993    −1.452974
H     4.139647     0.851242    −1.955292
H     6.243580     1.058744    −0.698127
C     2.260892    −1.182432    −2.564334
C     4.174992     1.508331    −1.079177
H     5.389681    −1.132894    −1.431462
H     1.496638    −0.446310    −2.820711
H     1.847780    −2.180105    −2.758244
C     5.293729     1.028410    −0.137554
H     2.283937     3.572905    −0.768687
C     4.991036    −1.425442    −0.452416
N     2.864239     1.568392    −0.460044
N     2.604484    −1.040694    −1.158151
H     3.607662    −2.849518    −1.299139
H     5.400049     1.737698     0.692776
C     2.436998     2.857115     0.050261
H     5.631945    −2.245439    −0.085180
N     5.093266    −0.284881     0.427175
C     3.570317    −1.984830    −0.624038
P     1.916873     0.204545    −0.270873
H     3.179947     3.277431     0.746048
H     1.488302     2.749711     0.578819
H     3.221278    −2.364478     0.342351
C     4.662593    −0.416008     1.798872
H     5.411926     0.030540     2.474807
H     3.391914     1.311762     2.015015
N     2.181505    −0.254142     1.338437
C     3.302033     0.225504     2.127408
H     4.630300    −1.486200     2.037649
C     1.358093    −1.297121     1.926929
H     0.585055    −1.591266     1.212016
H     3.072205     0.043397     3.186551
```

```
H        1.951309      −2.186269       2.194874
H        0.860050      −0.933833       2.837116
N        0.454161       0.576039      −0.725497
N       −0.454124      −0.573728      −0.727044
```

LA−6_N$_2$_LA−6
```
  108
xyz
 C       1.647518      −0.208294       0.244253
 N       3.655368       0.763570      −0.300377
 C       2.285773       0.984236      −0.148897
 N       3.900998      −0.587509       0.108156
 C       4.605740       1.672106       0.292286
 C       2.658397      −1.152443       0.384977
 C       4.814184      −1.270501      −0.771949
 N       1.757801       2.198058      −0.306735
 C       0.317335       2.501393      −0.100103
 C       2.454984       3.325906      −0.946072
 N       2.552349      −2.447339       0.708489
 C       1.240848      −3.091912       0.919749
 C       3.661144      −3.267740       1.209615
 C       4.363421      −1.814270      −1.973291
 C       6.150823      −1.361821      −0.402447
 C       5.264592      −2.469063      −2.806067
 C       6.608898      −2.566283      −2.443172
 C       7.052052      −2.009679      −1.245365
 C       5.674388       2.113236      −0.477927
 C       4.459948       2.076358       1.618000
 C       6.609556       2.981690       0.082467
 C       6.465043       3.403444       1.402328
 C       5.390205       2.950617       2.169484
 C       1.320225       4.276421      −1.336357
 C       0.265569       4.013977      −0.257642
 C       1.621411      −4.523544       1.290142
 C       2.952555      −4.348917       2.028679
 H       3.313645      −1.725740      −2.241173
 H       4.919632      −2.902503      −3.740202
 H       7.310129      −3.078077      −3.095790
 H       8.097651      −2.084793      −0.962032
 H       6.470455      −0.928993       0.540680
 H       5.759590       1.778290      −1.507239
 H       7.445871       3.332808      −0.514644
 H       7.189142       4.087083       1.835712
 H       5.277323       3.279589       3.198196
 H       3.616482       1.715266       2.200855
 H       3.044702       2.972972      −1.799242
 H       3.138170       3.806906      −0.236931
 H       1.659919       5.314871      −1.377629
 H       0.922782       4.007352      −2.321999
 H       0.545340       4.508874       0.680453
 H      −0.738056       4.349591      −0.529597
 H      −0.041292       2.124057       0.858983
 H      −0.271834       2.004904      −0.878777
 H       0.630271      −3.015544       0.016222
```

```
H      0.699073     −2.587073      1.724943
H      0.850610     −5.000604      1.900543
H      1.766073     −5.129362      0.387447
H      2.771099     −3.988998      3.047810
H      3.540121     −5.268815      2.089692
H      4.349425     −2.655449      1.801600
H      4.226046     −3.706236      0.377388
N      0.314138     −0.317931      0.653542
H     −0.985009     −3.251242      3.194870
H     −6.039618     −4.032734     −1.015519
C     −1.963516     −2.784486      3.371139
H     −2.636019     −3.573422      3.724890
C     −6.119560     −3.008111     −0.661536
H     −4.081967     −2.540112     −1.173351
H     −1.863137     −2.412098      1.214260
C     −1.813186     −1.633369      4.381668
C     −5.015111     −2.164416     −0.763504
C     −2.472020     −2.099781      2.084373
H     −8.161678     −3.219312     −0.003930
C     −7.305172     −2.556906     −0.089460
C     −1.503339     −0.442126      3.478380
N     −2.367089     −0.662923      2.333366
C     −2.328369      0.274975      1.257925
H     −3.512599     −2.371465      1.853940
H     −2.522755      2.574376      2.304906
C     −1.777232     −0.177831     −0.026190
C     −5.096945     −0.844541     −0.310004
N     −3.664139      0.755555      0.823511
C     −7.373724     −1.247516      0.389786
C     −2.796403     −0.290673     −0.990551
N     −4.013255      0.060095     −0.402883
H     −2.434471     −2.389275     −4.434819
C     −3.143878      3.017479      1.534943
C     −6.283096     −0.394630      0.281186
N     −2.767220     −0.607752     −2.293843
C     −1.554754     −1.026478     −2.994753
C     −3.793855      2.148802      0.640288
H     −4.637041     −1.149336     −3.130476
H     −8.286449     −0.885955      0.855579
C     −2.059298     −1.359151     −4.399155
H     −2.760064      5.041488      2.113123
C     −3.276543      4.393755      1.407710
C     −3.882023     −0.356960     −3.214376
H     −6.326809      0.617003      0.671628
C     −4.592913      2.713663     −0.366233
C     −3.214875     −0.370878     −4.590237
C     −4.057035      4.952993      0.392323
H     −4.363583      0.592617     −2.964807
H     −3.909594     −0.663401     −5.382364
H     −5.114662      2.065523     −1.062646
C     −4.715140      4.097960     −0.486814
H     −2.822862      0.624544     −4.830125
H     −4.157038      6.030967      0.297766
H     −5.335439      4.506021     −1.281809
```

```
H    −1.085410    −1.863832    −2.469272
H    −0.823419    −0.209004    −3.002880
H    −1.275157    −1.257547    −5.154720
H    −1.037270    −1.825858     5.131787
H    −0.432912    −0.425410     3.196353
H    −2.761687    −1.462936     4.904338
H    −1.740319     0.521220     3.943964
N    −0.492538    −0.381158    −0.368020
```

LA−4_LB−1
```
   13
xyz
N    −2.837935    −0.140369     0.277426
H    −3.752865     0.324845     0.269588
H    −2.794637    −1.146446     0.241748
N    −0.580710     0.014175    −0.236857
H     0.226467     0.590513    −0.421135
H    −0.395786    −0.834180     0.276806
N    −1.973375     1.885604    −0.389501
H    −1.146318     2.428240    −0.600096
C    −1.798933     0.602308    −0.115580
B    −3.314281     2.524612    −0.375675
N    −4.422729     3.084232    −1.153265
N    −4.232265     3.438541     0.310174
N    −4.690494     2.076016    −0.085554
```

LA−4_LB−2
```
   38
xyz
P    −0.282116    −0.145169     1.040304
C     0.113085     1.532219     0.473931
C    −0.406407     2.612274     1.196260
C     0.892073     1.755716    −0.664967
C    −0.155832     3.911698     0.765251
H    −0.988240     2.436137     2.097739
C     1.138138     3.058818    −1.088975
H     1.317195     0.919119    −1.213162
C     0.612201     4.134952    −0.376345
H    −0.553386     4.749886     1.329186
H     1.747091     3.232750    −1.971111
H     0.809783     5.150794    −0.706182
C     1.019727    −1.254147     0.435277
C     0.912924    −1.905379    −0.796872
C     2.160744    −1.425232     1.227043
C     1.954098    −2.715005    −1.242911
H     0.017017    −1.793305    −1.401859
C     3.196992    −2.235963     0.773449
H     2.228822    −0.940040     2.197697
C     3.095701    −2.877301    −0.460006
H     1.869417    −3.224541    −2.198148
H     4.079664    −2.373802     1.390332
H     3.904507    −3.513328    −0.807924
C    −1.840647    −0.641888     0.256515
C    −2.609415    −1.628125     0.884566
```

```
C   −2.262457   −0.083828   −0.953607
C   −3.790119   −2.062156    0.289296
H   −2.293380   −2.040027    1.839899
C   −3.445198   −0.523492   −1.542042
H   −1.679579    0.699935   −1.430222
C   −4.206025   −1.513499   −0.922750
H   −4.389937   −2.822798    0.779470
H   −3.775536   −0.086745   −2.479795
H   −5.130926   −1.851287   −1.381218
B   −0.412986   −0.212765    2.890229
N    0.352803   −0.178451    4.153003
N   −0.857865   −1.032295    4.035971
N   −0.993138    0.446919    4.078267
```

LA−4_LB−3
```
    44
xyz
P    0.037689   −0.096152    0.609561
C    0.029643    1.741944    0.133450
C    1.599409   −0.981770   −0.008561
C   −1.546807   −0.979996    0.049497
C    1.426944    2.346155    0.369573
H    2.175728    1.985720   −0.338814
H    1.349993    3.430774    0.229480
H    1.776480    2.170338    1.391321
C   −0.918746    2.496560    1.090673
H   −0.838606    3.567389    0.867552
H   −1.965750    2.220443    0.977872
H   −0.635577    2.349225    2.137124
C   −0.384010    1.989414   −1.325264
H   −0.291818    3.061790   −1.535855
H    0.251801    1.458941   −2.039869
H   −1.423147    1.712453   −1.519022
C    2.785989   −0.579830    0.894530
H    3.656781   −1.171995    0.588020
H    3.063558    0.469577    0.811961
H    2.583636   −0.799698    1.946994
C    1.438190   −2.503569    0.168610
H    0.707719   −2.940378   −0.515504
H    2.404753   −2.970229   −0.054786
H    1.176426   −2.765639    1.198106
C    1.927353   −0.679660   −1.478776
H    2.196930    0.366697   −1.641541
H    2.793247   −1.284839   −1.773451
H    1.105519   −0.931896   −2.155048
C   −1.542755   −1.346744   −1.442391
H   −2.516494   −1.783052   −1.695978
H   −1.393882   −0.478081   −2.090136
H   −0.783023   −2.092573   −1.688463
C   −1.735078   −2.249397    0.908792
H   −2.701347   −2.694768    0.642615
H   −0.972633   −3.008388    0.742080
H   −1.756773   −2.013175    1.976829
C   −2.769874   −0.091514    0.346019
```

```
H      −2.800236      0.218055      1.394975
H      −2.825897      0.790066     −0.295897
H      −3.670005     −0.686427      0.151646
B       0.072013     −0.173216      2.472429
N       0.650125      0.432286      3.691223
N       0.382326     −1.029955      3.636763
N      −0.750693     −0.067944      3.696483
```

LA−4_LB−4
```
    37
xyz
 P      −2.068634      1.446914      0.455980
 N      −3.549803      0.969185     −0.129287
 N      −1.042446      0.290852     −0.132557
 N      −1.740218      2.951740     −0.141521
 C      −4.020715     −0.403715      0.012972
 H      −4.846735     −0.469277      0.733194
 H      −3.211568     −1.052956      0.353037
 H      −4.377475     −0.772968     −0.956971
 C      −4.593019      1.932338     −0.452391
 H      −4.150216      2.872639     −0.783480
 H      −5.254234      2.123930      0.404521
 H      −5.198145      1.534480     −1.274758
 C      −1.103093     −0.171916     −1.514165
 H      −2.006501      0.195479     −2.004613
 H      −1.112351     −1.268622     −1.534398
 H      −0.228526      0.172288     −2.082528
 C       0.216718     −0.025621      0.546685
 H       0.156480      0.186210      1.614920
 H       1.048868      0.555721      0.131538
 H       0.421173     −1.093252      0.411842
 C      −2.191166      4.138156      0.595788
 H      −3.054132      3.902209      1.221030
 H      −2.477653      4.912547     −0.124976
 H      −1.392307      4.514704      1.245302
 C      −0.509390      3.199094     −0.896857
 H      −0.685459      4.037097     −1.579307
 H      −0.238681      2.330279     −1.497565
 H       0.314002      3.441555     −0.214367
 N      −2.035124      1.526635      2.081317
 C      −2.842234      0.646268      2.928003
 H      −3.874690      0.597120      2.568904
 H      −2.853061      1.065664      3.936071
 H      −2.428165     −0.368436      2.982268
 B      −0.847373      2.185703      2.679525
 N       0.381252      2.876909      2.258237
 N       0.400819      1.951834      3.429784
 N      −0.331916      3.272592      3.521972
```

LA−4_LB−5
```
    39
xyz
 P       8.691931     13.738298      4.608201
 N       6.729488     11.612394      4.223908
```

```
N      8.260893    13.072590    6.084000
N      7.416265    14.460388    3.781020
N      9.390874    12.532657    3.689116
C      6.812215    11.123376    5.578888
H      6.795435    10.023360    5.611407
H      5.932987    11.468232    6.132592
C      8.087320    11.641532    6.255741
H      8.077965    11.425207    7.329910
H      8.955603    11.123235    5.836796
C      7.499432    10.959574    3.195023
H      6.856356    10.652771    2.353213
H      7.923834    10.044019    3.622775
C      8.651118    11.834822    2.648014
H      9.360258    11.204595    2.101014
H      8.267740    12.559907    1.923088
C      5.721133    12.576105    3.874004
H      5.229131    12.892250    4.798006
H      4.940806    12.142951    3.221704
C      6.254991    13.817230    3.163710
H      6.473543    13.588089    2.109272
H      5.444547    14.557302    3.146567
C      7.644905    13.950844    7.072377
H      7.960459    13.648382    8.075921
C     10.733394    12.055963    4.011776
H     11.170997    12.671991    4.801633
C      7.687135    15.752908    3.135816
H      8.510921    16.275862    3.621146
H     10.716227    11.011374    4.352512
H     11.380686    12.130253    3.130927
H      6.546568    13.929725    7.019501
H      7.980314    14.979789    6.915181
H      6.791602    16.378768    3.211600
H      7.937430    15.621535    2.073829
B      9.947772    15.057994    4.990577
N     10.904026    16.069204    4.497691
N     11.245673    15.228318    5.679873
N     10.204376    16.272046    5.798230
```

LA−4_LB−6
```
    57
xyz
C      0.088738    −1.530338    −0.002529
N      0.621758     0.714330     0.176761
C      1.107948    −0.589261     0.236807
N     −0.750769     0.617916    −0.186868
C      1.316657     1.722980    −0.582580
C     −1.047232    −0.745716    −0.248033
C     −1.578832     1.504676     0.592626
N      2.406649    −0.786575     0.472936
C      3.050439    −2.118276     0.427814
C      3.300471     0.229145     1.049949
N     −2.309868    −1.112211    −0.494671
C     −2.762752    −2.515582    −0.473229
C     −3.320185    −0.221966    −1.086246
```

```
C     −1.980642      1.145399      1.877569
C     −1.944493      2.728413      0.044700
C     −2.772807      2.020188      2.613843
C     −3.146792      3.250546      2.071293
C     −2.729186      3.605975      0.790467
C      1.505219      2.976312     −0.012545
C      1.767621      1.445791     −1.871576
C      2.160446      3.968060     −0.739925
C      2.626738      3.696925     −2.024556
C      2.430611      2.435759     −2.589388
C      4.428305     −0.601212      1.662071
C      4.515549     −1.799036      0.712787
C     −4.251464     −2.401454     −0.792801
C     −4.310983     −1.191980     −1.729279
H     −1.678356      0.184921      2.286899
H     −3.097310      1.743171      3.612448
H     −3.765409      3.931229      2.648767
H     −3.019405      4.563025      0.367269
H     −1.616296      2.978865     −0.959588
H      1.143193      3.160947      0.994329
H      2.312332      4.948911     −0.299390
H      3.144970      4.467585     −2.587556
H      2.793552      2.224107     −3.590733
H      1.605310      0.459221     −2.297880
H      2.757259      0.838290      1.779608
H      3.687042      0.894791      0.269246
H      5.358988     −0.032323      1.736063
H      4.148472     −0.936503      2.667243
H      5.035967     −1.514099     −0.209587
H      5.035567     −2.656465      1.145995
H      2.879744     −2.592558     −0.539941
H      2.622661     −2.768302      1.196960
H     −2.550400     −2.973892      0.493762
H     −2.228173     −3.099210     −1.228451
H     −4.637387     −3.318140     −1.244608
H     −4.826517     −2.202313      0.119519
H     −3.968064     −1.473685     −2.731460
H     −5.309700     −0.756218     −1.818317
H     −2.849732      0.461461     −1.800419
H     −3.809758      0.378869     −0.310645
B      0.252936     −3.076563      0.014306
N      0.952544     −4.209472     −0.642561
N     −0.410526     −4.394256     −0.068969
N      0.754001     −4.204155      0.838445
```

LA−5a_LB−1
```
    42
xyz
C      0.598040     −0.243086     −1.387615
C      0.967957     −0.441541     −0.044525
C      2.079654     −1.200311      0.294695
H      2.345993     −1.343816      1.340197
C      2.851039     −1.788565     −0.712440
H      3.722224     −2.383843     −0.451858
```

```
C     2.490808    -1.621065    -2.045584
H     3.077497    -2.092513    -2.830538
C     1.367815    -0.853195    -2.375336
H     1.090130    -0.755030    -3.425374
C    -0.443522     2.013049    -0.633659
C    -0.019468     1.696211     0.670378
C     0.284099     2.687535     1.592681
H     0.606705     2.420854     2.597387
C     0.164923     4.032577     1.228017
H     0.401724     4.813001     1.946435
C    -0.268221     4.366753    -0.050751
H    -0.375473     5.411466    -0.332712
C    -0.572955     3.358081    -0.972661
H    -0.924889     3.641003    -1.964693
C    -1.842822    -0.135519    -0.610435
C    -1.368099    -0.351804     0.698081
C     0.030071     0.202830     0.969737
C    -2.133637    -1.019720     1.642180
H    -1.748391    -1.176392     2.647969
C    -3.404379    -1.492256     1.297101
H    -4.008029    -2.016015     2.033535
C    -3.890349    -1.289835     0.010485
H    -4.876983    -1.655993    -0.262704
C    -3.108180    -0.614413    -0.934179
H    -3.521059    -0.475414    -1.935311
H     0.349147     0.005901     1.998509
B    -0.750172     0.666132    -1.497666
N    -0.929517     1.463788    -5.235452
H     1.018344     2.004103    -2.733940
C    -0.518436     1.470593    -3.931157
N    -1.221709     0.932746    -2.970247
H    -0.653002     2.244324    -5.813653
N     0.670707     2.061918    -3.685346
H    -2.160508     0.649356    -3.222927
H     1.376320     2.023853    -4.406046
H    -1.845024     1.091864    -5.441069

LA–5a_LB–2
    67
xyz
P     1.118738     0.000240     0.001542
C     1.830979     1.476835     0.799039
C     1.148910     2.694450     0.696578
C     3.033458     1.414830     1.510061
C     1.677691     3.838823     1.285324
H     0.195061     2.747240     0.180703
C     3.557669     2.563190     2.098261
H     3.557685     0.469454     1.618895
C     2.882063     3.776217     1.983574
H     1.137717     4.777677     1.208503
H     4.490295     2.506479     2.651997
H     3.288516     4.670254     2.447706
C     1.832583    -1.428465     0.880840
C     3.033066    -2.014627     0.467811
```

```
C     1.153704    −1.947348     1.989100
C     3.558528    −3.098521     1.166884
H     3.554280    −1.637258    −0.407567
C     1.683680    −3.029740     2.684428
H     0.201540    −1.525655     2.296028
C     2.886119    −3.604569     2.277211
H     4.489530    −3.550855     0.837845
H     1.146191    −3.431718     3.537896
H     3.293404    −4.453875     2.818306
C     1.832264    −0.046403    −1.675514
C     1.154745    −0.749307    −2.678133
C     3.031388     0.606404    −1.977559
C     1.684850    −0.810826    −3.963047
H     0.203358    −1.227167    −2.465535
C     3.556920     0.542460    −3.265698
H     3.551588     1.177754    −1.213805
C     2.886005    −0.168766    −4.258140
H     1.148491    −1.351041    −4.737285
H     4.486871     1.055173    −3.493658
H     3.293369    −0.213432    −5.264120
H    −1.268658     1.463025     4.679732
C    −1.739006     1.169512     3.744531
H     0.137845     0.876760     2.764088
C    −0.942720     0.829862     2.645555
H    −3.745896     1.400530     4.492520
C    −3.124899     1.135815     3.640822
H     0.144498    −2.830252    −0.618883
H    −1.257091    −4.785658    −1.071064
C    −0.936391    −2.706567    −0.602479
C    −1.729822    −3.829880    −0.858894
C    −1.511180     0.450166     1.429401
C    −3.716210     0.759179     2.432478
C    −1.508003    −1.464575    −0.325018
C    −3.115973    −3.726022    −0.839006
C    −2.917108     0.422537     1.348458
B    −0.858721    −0.000551     0.000073
H    −3.734818    −4.597255    −1.036526
H    −4.800176     0.728618     2.340265
C    −3.710351    −2.492348    −0.562449
C    −2.913977    −1.383536    −0.310831
C    −3.473624    −0.001777    −0.003426
H    −4.794537    −2.399390    −0.544792
C    −1.508108     1.012518    −1.106066
H    −4.568436    −0.002354    −0.004938
C    −2.914113     0.956700    −1.045102
H     0.144016     1.955187    −2.137818
C    −0.936901     1.876540    −2.040740
C    −3.710805     1.728710    −1.879551
C    −1.730715     2.659874    −2.885313
H    −4.794973     1.664820    −1.809391
C    −3.116856     2.587678    −2.807456
H    −1.258327     3.323734    −3.605110
H    −3.735969     3.194225    −3.463082
```

LA–5a_LB–3
```
   73
xyz
  C      1.244619      0.311935      1.470201
  C      2.652748      0.312663      1.370782
  C      3.480147      0.560632      2.458049
  C      2.930407      0.816607      3.713873
  C      1.549659      0.799947      3.853032
  C      0.734948      0.545662      2.745742
  C      3.208346     -0.000253     -0.000112
  C      2.652536     -1.343786     -0.414590
  C      1.244443     -1.429502     -0.465036
  C      0.734846     -2.651170     -0.900149
  C      1.549564     -3.737268     -1.233490
  C      2.930332     -3.624978     -1.149607
  C      3.479956     -2.409371     -0.743438
  B      0.550634      0.000004     -0.000208
  P     -1.651855     -0.000065     -0.000118
  C     -2.398836     -1.470796      1.049207
  C     -2.364152     -2.844593      0.334960
  C      1.244704      1.117428     -1.005361
  C      2.652787      1.030693     -0.956308
  C      3.480414      1.848436     -1.714329
  C      2.930901      2.808535     -2.563481
  C      1.550168      2.937657     -2.618575
  C      0.735250      2.105686     -1.845124
  C     -2.399158      1.643971      0.749007
  C     -2.364370      1.712221      2.295926
  C     -2.398464     -0.173357     -1.798667
  C     -2.363418      1.132299     -2.630969
  C     -3.861633      1.901718      0.324886
  C     -1.556394      2.857133      0.308488
  C     -3.860928     -0.669325     -1.810031
  C     -1.555577     -1.161385     -2.628960
  C     -3.861258     -1.232043      1.484259
  C     -1.556289     -1.695676      2.320281
  H     -0.326351      2.272229     -1.899254
  H      1.093895      3.690206     -3.257395
  H      3.574016      3.449339     -3.160559
  H      4.560354      1.738184     -1.638394
  H      4.559915     -2.288546     -0.686139
  H      3.573369     -4.462631     -1.405649
  H      1.093170     -4.666941     -1.565160
  H     -0.326792     -2.781283     -1.016940
  H      4.560114      0.549816      2.324825
  H     -0.326684      0.509121      2.916801
  H      1.093275      0.977384      4.824025
  H      3.573402      1.013663      4.567364
  H      4.302854     -0.000374     -0.000165
  H     -0.491070      2.712026      0.503727
  H     -0.490144     -0.920415     -2.599936
  H     -0.490761     -1.790750      2.097475
  H     -1.886137     -1.086495     -3.672538
  H     -1.887779      3.723713      0.894275
```

```
H    −1.886762    −2.636940     2.777130
H    −1.686101     3.120048    −0.741057
H    −1.686291    −2.201872    −2.332693
H    −1.687542    −0.918798     3.073129
H    −1.380456     1.289241    −3.071806
H    −1.381880     2.016930     2.652397
H    −1.381492    −3.305408     0.419906
H    −3.067968     2.493517     2.606173
H    −3.065912     1.010080    −3.463623
H    −3.067279    −3.504038     0.856975
H    −4.161204    −2.078026     2.114559
H    −4.160629    −0.791706    −2.857953
H    −4.161437     2.870222     0.743265
H    −3.998546     1.974715    −0.752620
H    −3.997821    −0.334703     2.085264
H    −3.998158    −1.638643    −1.333951
H    −2.655940    −2.840212    −0.712988
H    −2.655344     0.802296     2.816221
H    −2.655626     2.037550    −2.103265
H    −4.558415    −1.190809     0.646226
H    −4.558031     0.035803    −1.355202
H    −4.558961     1.155151     0.707547
```

LA−5a_LB−4
```
   66
xyz
P    −2.298135    −0.062600    −0.112852
N    −3.574234    −0.813180    −0.891317
N    −2.744139     1.536564    −0.194896
N    −2.279316    −0.617198     1.440788
C    −4.078693    −0.359317    −2.180884
H    −3.742509    −1.015488    −2.994816
H    −3.732921     0.654051    −2.392792
H    −5.175905    −0.357624    −2.166088
C    −3.888395    −2.204913    −0.600380
H    −3.617181    −2.451323     0.427188
H    −3.364538    −2.894581    −1.278392
H    −4.967175    −2.360435    −0.716757
C    −4.108216     2.016588    −0.028517
H    −4.803422     1.182576     0.082878
H    −4.407748     2.604093    −0.906827
H    −4.187711     2.665820     0.854151
C    −1.756461     2.607225    −0.311296
H    −0.755985     2.205512    −0.463423
H    −1.743990     3.222881     0.596483
H    −2.010576     3.243467    −1.168377
C    −1.460372    −1.733946     1.899472
H    −0.859576    −2.135029     1.086714
H    −2.102354    −2.530317     2.301597
H    −0.775711    −1.390089     2.683066
C    −3.160611    −0.081571     2.464112
H    −4.000150    −0.761829     2.665768
H    −3.558701     0.891602     2.175211
H    −2.590107     0.053568     3.390792
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                          96
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```
N      −0.866369     −0.342640     −0.796304
C      −0.919434     −0.821668     −2.191527
H      −1.499488     −1.746992     −2.281737
H       0.098688     −1.034833     −2.515359
H      −1.338749     −0.078437     −2.880001
H      −0.071759      2.266760      4.043575
C       0.604380      1.795917      3.332956
H      −0.979888      1.292244      2.007418
C       0.090997      1.229303      2.161343
H       2.376248      2.196133      4.495371
C       1.969660      1.762750      3.585397
H       0.090759      1.635978     −2.673605
H       1.743054      2.962520     −3.923767
C       1.131301      1.612800     −2.353650
C       2.064524      2.372809     −3.068223
C       0.905487      0.607233      1.211815
C       2.817041      1.183284      2.639515
C       1.508393      0.844482     −1.253002
C       3.401219      2.374213     −2.685204
C       2.294644      0.631263      1.477167
B       0.613217     −0.101133     −0.250921
H       4.130406      2.960395     −3.238480
H       3.892866      1.174621      2.804410
C       3.801088      1.622921     −1.576033
C       2.863842      0.877317     −0.875133
C       3.189185      0.074399      0.378538
H       4.842505      1.628697     −1.259067
C       1.426171     −1.522296     −0.209075
H       4.248035      0.155788      0.646159
C       2.779213     −1.365311      0.130223
H      −0.061076     −2.982858     −0.765663
C       0.977148     −2.814908     −0.477666
C       3.643883     −2.448388      0.219176
C       1.834408     −3.917231     −0.395350
H       4.687430     −2.295019      0.488521
C       3.168465     −3.735912     −0.043327
H       1.459263     −4.915459     −0.609523
H       3.839099     −4.588806      0.022187
```

LA−5a_LB−5
```
    68
xyz
 P      1.193613      0.000259      0.000237
 N      4.451273      0.000152     −0.000013
 N      1.833553     −1.211957      0.965317
 N      1.833836     −0.229332     −1.531821
 N      1.833400      1.442125      0.567227
 C      4.349814     −1.004812      1.030478
 H      5.156039     −0.874247      1.771467
 H      4.510651     −1.984828      0.565776
 C      3.015378     −1.006868      1.790868
 H      3.030164     −1.799278      2.549227
 H      2.917869     −0.059962      2.333790
 C      4.349544      1.395064      0.354950
```

```
H      5.155700      1.971558     −0.128661
H      4.510308      1.482820      1.436011
C      3.014975      2.054334     −0.023696
H      3.029679      3.107528      0.282583
H      2.917022      2.049940     −1.115177
C      4.349613     −0.389977     −1.385510
H      5.155945     −1.096802     −1.643114
H      4.509903      0.502459     −2.002037
C      3.015059     −1.047668     −1.766647
H      3.029368     −1.309416     −2.831786
H      2.917114     −1.990451     −1.216676
C      1.265016     −2.553324      0.944896
H      0.313806     −2.557286      0.409357
C      1.265867      2.094666      1.739778
H      0.315704      1.631671      2.012673
C      1.267065      0.460127     −2.683433
H      0.318767      0.931412     −2.418433
H      1.940136      2.034494      2.606249
H      1.064776      3.150173      1.521876
H      1.065613     −2.892419      1.968253
H      1.937839     −3.274037      0.458158
H      1.062897     −0.256535     −3.487649
H      1.943491      1.237993     −3.066059
H     −1.192605      4.695503     −1.415903
C     −1.662715      3.757170     −1.130969
H      0.213970      2.767867     −0.827963
C     −0.867866      2.655428     −0.796963
H     −3.669311      4.508637     −1.357002
C     −3.048793      3.654550     −1.098856
H      0.214425     −0.663857      2.811163
H     −1.191593     −1.119963      4.774461
C     −0.867433     −0.636149      2.698104
C     −1.661942     −0.898439      3.819297
C     −1.435817      1.435475     −0.427302
C     −3.640247      2.443106     −0.732777
C     −1.435691     −0.347482      1.456642
C     −3.048050     −0.876579      3.714265
C     −2.841681      1.355892     −0.404741
B     −0.771760      0.000248     −0.000009
H     −3.668396     −1.080565      4.582998
H     −4.724316      2.350381     −0.705736
C     −3.639805     −0.588686      2.482021
C     −2.841544     −0.328476      1.376379
C     −3.400239     −0.000643     −0.000550
H     −4.723901     −0.566775      2.388219
C     −1.434956     −1.087711     −1.029520
H     −4.495138     −0.000993     −0.000808
C     −2.840820     −1.028799     −0.972841
H      0.215995     −2.100651     −1.981208
C     −0.865974     −2.017863     −1.900456
C     −3.638507     −1.856860     −1.750901
C     −1.659887     −2.858333     −2.688132
H     −4.722653     −1.787406     −1.684993
C     −3.046060     −2.779534     −2.616441
```

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H     -1.189029    -3.574260    -3.357743
H     -3.665905    -3.430393    -3.227438
```

LA−5a_LB−6
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    86
xyz
C     -0.041618    -0.041243     0.329761
N     -2.220051     0.797486     0.274414
C     -0.879760     1.042791     0.639710
N     -2.249791    -0.564019    -0.141622
C     -2.832640     1.669163    -0.704971
C     -0.960794    -1.062221     0.037374
C     -3.403146    -1.251993     0.369394
N     -0.581964     2.197507     1.240815
C      0.610192     2.360509     2.092987
C     -1.547983     3.280295     1.463908
N     -0.770770    -2.387780    -0.035706
C      0.354570    -3.082884     0.613294
C     -1.569527    -3.294848    -0.870528
C     -3.411316    -1.742744     1.674003
C     -4.508394    -1.408994    -0.458624
C     -4.535264    -2.412397     2.145246
C     -5.649382    -2.575564     1.320078
C     -5.637660    -2.069533     0.022239
C     -4.130907     2.112688    -0.483901
C     -2.139983     2.022301    -1.861829
C     -4.743255     2.935142    -1.427420
C     -4.052771     3.309599    -2.578724
C     -2.752350     2.852572    -2.795349
C     -0.897630     4.151552     2.545082
C      0.597343     3.848909     2.403179
C      0.084243    -4.555195     0.298162
C     -0.641930    -4.495558    -1.049051
H     -2.535868    -1.606923     2.303618
H     -4.544403    -2.806329     3.157303
H     -6.525698    -3.099236     1.690759
H     -6.503414    -2.196105    -0.621026
H     -4.470121    -1.019615    -1.471456
H     -4.645580     1.814282     0.424642
H     -5.756897     3.287092    -1.259748
H     -4.527928     3.957414    -3.309592
H     -2.213754     3.139905    -3.693392
H     -1.132108     1.647583    -2.024607
H     -2.515359     2.870357     1.774934
H     -1.702214     3.838051     0.533028
H     -1.142590     5.208788     2.414672
H     -1.248478     3.844000     3.536913
H      1.030867     4.399618     1.560243
H      1.171709     4.086269     3.301960
H      1.513856     2.031661     1.588818
H      0.478995     1.754802     3.000340
H      0.358368    -2.860489     1.683363
H      1.308103    -2.758123     0.194770
H      1.010701    -5.132923     0.259484
```

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H     -0.566981     -5.001824      1.059532
H      0.076273     -4.298944     -1.851810
H     -1.194565     -5.409114     -1.285442
H     -1.836271     -2.800468     -1.810666
H     -2.495966     -3.591303     -0.363362
H      2.608985     -1.431544      4.597621
C      2.959720     -1.193462      3.595526
H      0.986737     -0.768753      2.847863
C      2.048694     -0.818489      2.603588
H      5.032845     -1.553916      4.066748
C      4.319547     -1.261812      3.300061
H      0.646864      2.730668     -0.845922
H      2.051585      4.563327     -1.667463
C      1.721289      2.572968     -0.902267
C      2.516816      3.626381     -1.367610
C      2.468579     -0.508195      1.310724
C      4.763913     -0.948311      2.013227
C      2.273348      1.354319     -0.501973
C      3.896180      3.475779     -1.450518
C      3.843315     -0.574879      1.040538
B      1.567267     -0.046669      0.031493
H      4.520151      4.291559     -1.806495
H      5.825403     -0.993252      1.775071
C      4.472017      2.252075     -1.097042
C      3.670483      1.211871     -0.647217
C      4.208715     -0.191997     -0.378994
H      5.546730      2.107470     -1.193759
C      2.036145     -1.002680     -1.231185
H      5.288874     -0.247668     -0.552829
C      3.438882     -1.086913     -1.344183
H      0.201808     -1.510369     -2.244544
C      1.284799     -1.614350     -2.235225
C      4.051607     -1.832116     -2.342832
C      1.888105     -2.357677     -3.255601
H      5.137847     -1.880465     -2.397786
C      3.271890     -2.491073     -3.297694
H      1.272776     -2.824269     -4.022551
H      3.745922     -3.072929     -4.084058

LA-5b_LB-5
    68
xyz
 C     -3.511263      0.901800      3.734805
 C     -3.939696      0.591461      2.443030
 C     -3.010575      0.348971      1.432559
 C     -1.624210      0.413710      1.701561
 C     -1.221931      0.724638      3.001584
 C     -2.150014      0.968933      4.017488
Al     -0.746283     -0.004343     -0.010001
 C     -1.641834      1.268277     -1.214913
 C     -1.253530      2.240053     -2.138741
 C     -2.192495      2.996859     -2.844872
 C     -3.550581      2.783288     -2.627165
 C     -3.965066      1.818282     -1.707657
```

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C    −3.025266     1.065147    −1.005674
C    −3.490661     0.004406     0.009995
C    −3.028873    −1.405033    −0.406361
C    −1.646148    −1.685929    −0.496149
C    −1.261168    −2.971580    −0.880137
C    −2.202710    −3.963203    −1.168577
C    −3.560046    −3.669797    −1.074097
C    −3.971211    −2.391224    −0.693781
P     1.658238    −0.004465    −0.008850
N     2.273881    −0.961083    −1.241877
C     1.664982    −0.883788    −2.563987
N     2.266142     1.545181    −0.217808
C     1.649546     2.648799     0.508303
N     2.263654    −0.594355     1.440115
C     1.650399    −1.777262     2.031480
C     3.459803     1.828858    −1.001318
C     4.775669     1.402779    −0.333751
N     4.821845     0.001484     0.002789
C     4.772290    −0.407856     1.384391
C     3.451520    −0.050254     2.081905
C     4.782448    −0.990412    −1.042916
C     3.466682    −1.781209    −1.087728
H     5.604655     1.670448    −1.010387
H     4.924608     1.979758     0.586370
H     3.477636     2.905931    −1.205211
H     3.378645     1.328490    −1.973756
H     5.610144    −1.710844    −0.930489
H     4.938766    −0.482082    −2.001522
H     3.490448    −2.496078    −1.918616
H     3.378887    −2.373351    −0.168889
H     5.596203     0.049317     1.957875
H     4.927491    −1.492312     1.424840
H     3.467699    −0.411569     3.116868
H     3.363468     1.041634     2.133747
H     0.731341     2.315209     1.003487
H     0.739303    −0.299545    −2.524624
H     0.732211    −2.040301     1.495403
H     2.331783    −0.403304    −3.293441
H     1.406216    −1.885517    −2.925508
H     1.376784     3.456111    −0.180913
H     2.318119     3.051255     1.281950
H     1.377676    −1.585862     3.075558
H     2.320786    −2.647055     1.991834
H    −1.879307    −4.958352    −1.465311
H    −0.201043    −3.216602    −0.961072
H    −4.301590    −4.433127    −1.296030
H    −0.192682     2.421099    −2.318627
H    −1.866486     3.748477    −3.560269
H    −4.290129     3.366075    −3.170548
H    −5.034267    −2.166672    −0.622475
H    −5.028654     1.655927    −1.540329
H    −4.585846     0.007804     0.017495
H    −0.158406     0.778625     3.239513
H    −5.005704     0.539325     2.227418
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H      −1.813194      1.209885      5.023227
H      −4.242467      1.089781      4.517003
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LA−5b_LB−6
```
   86
xyz
C       3.270709     −2.643720     −3.440260
C       4.003883     −1.790221     −2.614229
C       3.381862     −1.114678     −1.564814
C       2.004420     −1.289300     −1.301697
C       1.294060     −2.130948     −2.162205
C       1.906268     −2.807351     −3.221089
Al      1.531334     −0.150826      0.274388
C       2.274773      1.548953     −0.492888
C       1.778200      2.834070     −0.738385
C       2.552726      3.835062     −1.331891
C       3.867587      3.559963     −1.693764
C       4.390029      2.284816     −1.472515
C       3.607726      1.289144     −0.888170
C       4.186758     −0.123812     −0.710122
C       4.225983     −0.543399      0.765280
C       3.016559     −0.632500      1.488273
C       3.090288     −1.017835      2.829589
C       4.309367     −1.308543      3.448600
C       5.490293     −1.214881      2.716996
C       5.446551     −0.832091      1.375404
C      −0.396967     −0.162205      0.835896
C      −1.174140      1.000259      0.915807
N      −2.461979      0.831307      0.380177
N      −2.525903     −0.542228     −0.006841
C      −1.315867     −1.114636      0.365949
C      −2.868576      1.714005     −0.691702
C      −4.169377      2.203214     −0.696984
C      −4.579660      3.041766     −1.731617
C      −3.686050      3.389400     −2.743141
C      −2.382683      2.891350     −2.729076
C      −1.970661      2.043072     −1.706361
N      −0.829770      2.179281      1.436392
C       0.375411      2.321475      2.273789
C       0.355438      3.795643      2.662174
C      −1.139459      4.117620      2.745465
C      −1.736221      3.324952      1.579856
C      −3.795029     −1.144180      0.292880
C      −4.085482     −1.562557      1.590345
C      −5.316723     −2.150877      1.858736
C      −6.254951     −2.304976      0.836586
C      −5.961520     −1.870154     −0.454057
C      −4.725027     −1.289173     −0.729814
N      −1.141771     −2.438085      0.297416
C      −0.001425     −3.102029      0.953344
C      −0.316847     −4.585293      0.771315
C      −1.038968     −4.616216     −0.579990
C      −1.926078     −3.370209     −0.524363
H      −3.343176     −1.433477      2.373722
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H    −5.546581    −2.488654     2.864955
H    −7.215507    −2.765235     1.048675
H    −6.691503    −1.988498    −1.249209
H    −4.468703    −0.952202    −1.729622
H    −4.844103     1.927842     0.108265
H    −5.594352     3.428674    −1.742303
H    −4.004206     4.050619    −3.543855
H    −1.683546     3.160558    −3.514978
H    −0.958090     1.645709    −1.691394
H    −2.756190     2.978922     1.774930
H    −1.747627     3.913256     0.654515
H    −1.358593     5.185536     2.666779
H    −1.551242     3.755036     3.694566
H     0.835419     4.387766     1.874515
H     0.889314     3.978072     3.597735
H     1.278233     2.052932     1.725497
H     0.283496     1.657436     3.143760
H     0.061676    −2.781684     1.997121
H     0.936683    −2.842980     0.453171
H     0.589625    −5.194706     0.784376
H    −0.982298    −4.939206     1.568081
H    −0.309950    −4.527047    −1.392052
H    −1.624916    −5.525550    −0.737982
H    −2.124384    −2.929950    −1.507484
H    −2.887775    −3.595742    −0.049390
H     4.338165    −1.605932     4.494794
H     2.174046    −1.095233     3.417113
H     6.445344    −1.438224     3.186535
H     0.751190     3.078019    −0.460462
H     2.131398     4.822653    −1.509617
H     4.484984     4.328872    −2.151793
H     6.372057    −0.759544     0.805731
H     5.416012     2.066702    −1.765497
H     5.216705    −0.114653    −1.084519
H     0.221356    −2.262675    −2.016489
H     5.067781    −1.647146    −2.797933
H     1.321463    −3.453124    −3.873537
H     3.763319    −3.166223    −4.256670
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LA−5d_LB−1
```
    41
xyz
 C    −3.076347    −0.600616    −0.956128
 C    −1.817798    −0.147113    −0.560174
 C    −1.473832    −0.422724     0.767504
 C    −2.280171    −1.092085     1.677548
 C    −3.530444    −1.525187     1.239691
 C    −3.920979    −1.277914    −0.073063
 B    −0.693759     0.654694    −1.425474
 N    −1.160376     0.923778    −2.886929
 C    −0.481841     1.480255    −3.872303
 N     0.715502     2.050210    −3.657213
 S     0.152613     0.150655     1.289891
 C     0.033108     1.855917     0.738062
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C    −0.404343     2.024152    −0.577659
C    −0.586795     3.347971    −0.984897
C    −0.318525     4.416291    −0.125540
C     0.134457     4.193266     1.172591
C     0.307473     2.887045     1.626545
C     1.129565    −0.539015    −0.051278
C     0.648938    −0.275665    −1.336034
C     1.350799    −0.890453    −2.375720
C     2.469634    −1.688464    −2.126784
C     2.920442    −1.901653    −0.826014
C     2.235055    −1.326882     0.242131
N    −0.958202     1.497941    −5.137506
H     2.553454    −1.498201     1.266287
H     3.790240    −2.522927    −0.639764
H     2.990493    −2.155923    −2.957356
H     1.014277    −0.767432    −3.402424
H     0.638716     2.688323     2.641645
H     0.339933     5.027863     1.834771
H    −0.472375     5.434174    −0.471649
H    −0.958123     3.559633    −1.984717
H    −1.953019    −1.275041     2.696890
H    −4.190530    −2.051798     1.920846
H    −4.894092    −1.616091    −0.416380
H    −3.432164    −0.438234    −1.971954
H     1.113566     2.029023    −2.728202
H    −0.599804     2.158516    −5.810943
H    −2.104627     0.654964    −3.131942
H     1.355937     2.198537    −4.422357
H    −1.848429     1.076550    −5.355210

LA−5d_LB−2
    66
xyz
C    −2.893428    −1.875511     3.485788
C    −3.571900    −1.296964     2.416687
C    −2.814641    −0.744174     1.391672
C    −1.416150    −0.716116     1.338419
C    −0.779724    −1.310890     2.433740
C    −1.501855    −1.879048     3.485006
B    −0.786342     0.000001    −0.000067
C    −1.416556     1.517012    −0.049104
C    −0.780396     2.763100    −0.082178
C    −1.502845     3.957434    −0.115329
C    −2.894413     3.956004    −0.118039
C    −3.572604     2.740703    −0.084379
C    −2.815079     1.576789    −0.050929
S    −3.665839    −0.000197     0.000510
C    −2.815197    −0.832926    −1.339706
C    −1.416679    −0.800993    −1.289276
C    −0.780657    −1.452000    −2.352367
C    −1.503179    −2.078000    −3.369972
C    −2.894748    −2.080281    −3.366837
C    −3.572822    −1.443923    −2.330835
P     1.211832    −0.000175    −0.000248
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C      1.912216      0.435261      1.622969
C      1.272354      1.388828      2.423754
C      1.814978      1.740555      3.655012
C      2.993641      1.142102      4.097709
C      3.628111      0.185859      3.308413
C      3.089956     −0.170146      2.074106
C      1.912152     −1.623684     −0.434730
C      1.271520     −2.794098     −0.010709
C      1.814217     −4.036174     −0.322058
C      2.993668     −4.120164     −1.060444
C      3.628993     −2.958363     −1.492329
C      3.090776     −1.711521     −1.183235
C      1.912273      1.187930     −1.188842
C      3.089753      1.881625     −0.889833
C      3.627671      2.773129     −1.814879
C      2.993238      2.978821     −3.037640
C      1.814973      2.295729     −3.334983
C      1.272568      1.404699     −2.415160
H      0.339262     −2.745717      0.542808
H      3.587463     −0.812274     −1.535763
H      1.309377     −4.939666      0.005588
H      4.543187     −3.019284     −2.074605
H      3.412952     −5.091322     −1.305092
H      3.585724      1.738247      0.065719
H      0.341113      0.899989     −2.650648
H      4.541007      3.309022     −1.575812
H      1.310780      2.462812     −4.281759
H      3.412314      3.676580     −3.756191
H      0.340478      1.844402      2.104613
H      3.585841     −0.926137      1.472278
H      1.310664      2.476880      4.273044
H      4.541652     −0.288773      3.652932
H      3.412907      1.415955      5.061050
H     −0.966026     −2.571964     −4.174287
H      0.302488     −1.490502     −2.403822
H     −3.449562     −2.570125     −4.160213
H      0.302740      2.826755     −0.090740
H     −0.965653      4.900941     −0.141562
H     −3.449088      4.888098     −0.145495
H     −4.658441     −1.426552     −2.301566
H     −4.658224      2.706805     −0.083434
H      0.303416     −1.335899      2.492588
H     −4.657528     −1.280514      2.387320
H     −0.964396     −2.328171      4.314998
H     −3.447898     −2.317449      4.307047

LA−5d_LB−3
    72
xyz
C     −2.679285     −2.134041      3.320717
C     −3.330630     −1.451984      2.298116
C     −2.556615     −0.833618      1.323982
C     −1.154447     −0.825781      1.266298
C     −0.561195     −1.544222      2.303640
```

```
C   -1.290728   -2.179242    3.309536
B   -0.476738   -0.000038    0.000098
C   -1.154159    1.509578    0.081864
C   -0.560588    2.766971    0.184996
C   -1.289621    3.955891    0.231792
C   -2.678183    3.943494    0.187231
C   -3.329960    2.717043    0.108170
C   -2.556282    1.563953    0.059856
S   -3.409814    0.000375   -0.000240
C   -2.556334   -0.729598   -1.384365
C   -1.154192   -0.683801   -1.348219
C   -0.560646   -1.223702   -2.488501
C   -1.289862   -1.777535   -3.541500
C   -2.678449   -1.809320   -3.508596
C   -3.330125   -1.264198   -2.407060
P    1.729678   -0.000038    0.000030
C    2.470296    1.199410   -1.365373
C    2.484932    2.705459   -0.979929
C    2.469816    0.582801    1.721615
C    3.923079    1.092966    1.589056
C    2.470287   -1.782247   -0.355902
C    3.923408   -1.922555    0.152791
C    2.484512   -0.504188    2.833015
C    1.619646    1.721942    2.319319
C    1.619733   -2.869460    0.331343
C    2.485759   -2.201209   -1.852999
C    3.923814    0.829599   -1.740076
C    1.620504    1.147253   -2.650994
H    3.301109   -0.263307    3.521541
H    1.567893   -0.478355    3.422150
H    2.652272   -1.525665    2.501033
H    1.961047    1.883752    3.348401
H    1.736256    2.674934    1.803633
H    0.556578    1.470105    2.362952
H    4.225671    1.475877    2.570241
H    4.629302    0.307133    1.319428
H    4.042919    1.915458    0.887621
H    1.961049   -3.841554   -0.043193
H    1.735954   -2.899708    1.414527
H    0.556704   -2.781117    0.091278
H    3.302739   -2.917576   -1.988317
H    1.569511   -2.724738   -2.125599
H    2.653399   -1.402907   -2.571572
H    4.043369   -1.724793    1.215506
H    4.225428   -2.964146   -0.004578
H    4.630174   -1.297473   -0.393772
H    4.226573    1.487085   -2.562848
H    4.629560    0.990080   -0.924490
H    4.044173   -0.189481   -2.100340
H    1.961997    1.957478   -3.305721
H    1.737105    0.224052   -3.218290
H    0.557384    1.310909   -2.454944
H    2.653094    2.928992    0.070593
H    3.301305    3.181172   -1.533237
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H      1.568227     3.202660    -1.296723
H     -0.759081    -2.182721    -4.398311
H      0.508540    -1.202671    -2.579997
H     -3.247950    -2.239289    -4.325699
H      0.508557     2.835623     0.249794
H     -0.758722     4.900409     0.309751
H     -3.247581     4.866175     0.223345
H     -4.414758    -1.254627    -2.349347
H     -4.414594     2.662384     0.087244
H      0.507935    -1.634954     2.330930
H     -4.415246    -1.406348     2.260969
H     -0.760212    -2.719372     4.088544
H     -3.249036    -2.626684     4.101455
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LA-5d_LB-4
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   65
xyz
C      2.881425    -3.926159    -0.121859
C      3.477917    -2.695807     0.136370
C      2.672410    -1.564176     0.076556
C      1.309807    -1.550716    -0.215421
C      0.756642    -2.809738    -0.473578
C      1.522405    -3.974788    -0.427278
B      0.537147    -0.093111    -0.242702
C      1.417185     0.855268    -1.273635
C      0.955088     1.632964    -2.340051
C      1.819537     2.405883    -3.117223
C      3.187068     2.432846    -2.855178
C      3.691580     1.690046    -1.790841
C      2.792629     0.937552    -1.045629
S      3.387615     0.042725     0.393335
C      2.201774     0.675507     1.582688
C      0.845805     0.623267     1.220126
C      0.001001     1.264809     2.134957
C      0.469853     1.852136     3.311285
C      1.822215     1.835167     3.633539
C      2.712873     1.244876     2.742883
N     -0.936600    -0.307340    -0.765333
C     -1.008938    -0.792325    -2.164559
P     -2.401917    -0.046990    -0.100826
N     -2.369051    -0.545519     1.471348
C     -3.316560    -0.019928     2.447182
N     -3.630173    -0.853530    -0.876093
C     -3.941115    -2.237744    -0.534332
N     -2.869688     1.536688    -0.236019
C     -1.909169     2.634297    -0.317416
C     -4.165136    -0.439060    -2.170866
C     -4.254603     1.988738    -0.119112
C     -1.584636    -1.668810     1.972631
H     -3.839219    -1.119083    -2.967885
H     -3.834115     0.570104    -2.420599
H     -5.260388    -0.446634    -2.132820
H     -3.680855    -2.448583     0.503422
H     -3.410726    -2.946929    -1.185284
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107
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H    -5.017192    -2.400418    -0.653841
H    -4.932608     1.142996     0.002185
H    -4.543038     2.541537    -1.021402
H    -4.368308     2.659708     0.741631
H    -0.893880     2.259377    -0.433650
H    -1.948708     3.252951     0.587541
H    -2.148559     3.264467    -1.182016
H    -0.950610    -2.080139     1.191444
H    -2.246098    -2.460262     2.348722
H    -0.940117    -1.328759     2.791426
H    -4.167019    -0.699552     2.588938
H    -3.692977     0.957929     2.145669
H    -2.803498     0.100071     3.407970
H    -1.576842    -1.724470    -2.241896
H     0.001249    -0.992348    -2.519482
H    -1.458913    -0.059497    -2.842860
H    -0.237129     2.332997     3.981766
H    -1.061434     1.313344     1.942300
H     2.183712     2.287969     4.550815
H    -0.104529     1.645837    -2.576051
H     1.419213     2.995024    -3.937351
H     3.855010     3.032528    -3.464690
H     3.780089     1.238861     2.945219
H     4.750960     1.705862    -1.551317
H    -0.298146    -2.890999    -0.722494
H     4.535427    -2.625721     0.374417
H     1.053959    -4.932779    -0.634305
H     3.472709    -4.835300    -0.087753

LA-5d_LB-5
    67
xyz
  C    -2.813861    -3.746160    -1.274640
  C    -3.488769    -2.592261    -0.886985
  C    -2.728858    -1.490573    -0.513960
  C    -1.330433    -1.434186    -0.494230
  C    -0.698397    -2.619246    -0.889969
  C    -1.422242    -3.750471    -1.271193
  B    -0.685228    -0.000037     0.000088
  C    -1.330550     0.288972     1.489072
  C    -0.698436     0.538600     2.713224
  C    -1.422212     0.774000     3.883539
  C    -2.813838     0.769109     3.881494
  C    -3.488819     0.528307     2.688288
  C    -2.728946     0.300434     1.547688
  S    -3.579696     0.000133    -0.000267
  C    -2.728683     1.190388    -1.034214
  C    -1.330258     1.145197    -0.994795
  C    -0.698025     2.080722    -1.822804
  C    -1.421742     2.976510    -2.611953
  C    -2.813351     2.977131    -2.607041
  C    -3.488440     2.064255    -1.801981
  P     1.312721     0.000178     0.000141
  N     1.916867     1.554728    -0.105906
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C      1.377380      2.630479      0.719166
N      1.916512     -0.685159      1.399446
C      1.376454     -1.937145      1.918872
N      1.916514     -0.869056     -1.293095
C      1.376780     -0.693195     -2.637270
C      3.109432     -0.164262      2.067503
C      4.430747     -0.483880      1.356112
N      4.471395     -0.000337     -0.000276
C      4.430511     -0.933302     -1.097095
C      3.108904     -1.708695     -1.175651
C      4.430872      1.416078     -0.259773
C      3.109381      1.872648     -0.891672
H      5.251356     -0.055792      1.953285
H      4.591043     -1.567842      1.341044
H      3.121578     -0.574806      3.083574
H      3.016263      0.921967      2.171823
H      5.251160      1.718929     -0.929592
H      4.591828      1.945033      0.686391
H      3.121727      2.957857     -1.044180
H      3.015503      1.419715     -1.884431
H      5.250842     -1.664791     -1.024662
H      4.591077     -0.378539     -2.028447
H      3.120751     -2.383742     -2.038941
H      3.015416     -2.341655     -0.286728
H      0.420832     -2.170977      1.446690
H      0.421067      2.339341      1.156823
H      0.421763     -0.166253     -2.604524
H      2.059841      2.902878      1.535142
H      1.199025      3.518648      0.102807
H      1.196538     -1.846592      2.995907
H      2.059340     -2.779980      1.748371
H      1.195954     -1.671333     -3.096739
H      2.060464     -0.125332     -3.282155
H     -0.887042      3.683927     -3.239263
H      0.385549      2.121857     -1.855954
H     -3.369691      3.676762     -3.221996
H      0.385118      0.547324      2.765398
H     -0.887602      0.963760      4.809865
H     -3.370285      0.951772      4.794842
H     -4.574013      2.037337     -1.777816
H     -4.574388      0.520724      2.652805
H      0.385153     -2.668995     -0.908473
H     -4.574336     -2.557650     -0.875951
H     -0.887651     -4.647656     -1.569767
H     -3.370334     -4.628480     -1.573022

LA−5d_LB−6
   85
xyz
C      3.105412     -2.611191     -3.289354
C      3.946375     -1.982420     -2.375087
C      3.359627     -1.204190     -1.384183
C      1.985276     -1.014176     -1.205605
C      1.187886     -1.605020     -2.192560
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C      1.731930    -2.392287    -3.207737
B      1.518151    -0.009954     0.026839
C      2.192788     1.381379    -0.578553
C      1.556847     2.529849    -1.065329
C      2.272761     3.605079    -1.593863
C      3.662945     3.574690    -1.668752
C      4.338975     2.434590    -1.242052
C      3.585505     1.387369    -0.726136
S      4.421713    -0.167967    -0.366787
C      3.769442    -0.510060     1.258878
C      2.384780    -0.406800     1.360529
C      1.869792    -0.647162     2.639260
C      2.695247    -0.970872     3.714511
C      4.078069    -1.067768     3.551251
C      4.636342    -0.831956     2.299281
C     -0.087483    -0.007976     0.315096
C     -0.947716     1.074579     0.596256
N     -2.274606     0.765728     0.278264
N     -2.274832    -0.597973    -0.102744
C     -0.987544    -1.066435     0.068130
C     -3.031362     1.598676    -0.631066
C     -4.328906     1.958318    -0.289043
C     -5.074969     2.736738    -1.171203
C     -4.518986     3.147461    -2.381410
C     -3.219060     2.770736    -2.720479
C     -2.472676     1.985465    -1.847378
N     -0.670429     2.268715     1.135942
C      0.516434     2.497327     1.980458
C      0.456076     3.992302     2.250741
C     -1.045507     4.239709     2.415043
C     -1.687003     3.308508     1.379542
C     -3.445535    -1.305640     0.340437
C     -3.531224    -1.754533     1.656626
C     -4.667048    -2.443627     2.067774
C     -5.712524    -2.664534     1.169410
C     -5.623414    -2.196243    -0.139650
C     -4.482931    -1.514605    -0.559977
N     -0.759926    -2.390466     0.020538
C      0.349646    -3.054785     0.723905
C      0.082046    -4.541792     0.481457
C     -0.626197    -4.552070    -0.875883
C     -1.555535    -3.345478    -0.768866
H     -2.709176    -1.571112     2.343588
H     -4.740314    -2.806102     3.088557
H     -6.598404    -3.202194     1.493170
H     -6.438447    -2.365299    -0.836450
H     -4.387751    -1.148753    -1.577812
H     -4.741013     1.631041     0.660769
H     -6.088993     3.024102    -0.911300
H     -5.100280     3.759217    -3.064430
H     -2.789467     3.083854    -3.667168
H     -1.465813     1.666230    -2.106098
H     -2.613377     2.853744     1.745045
H     -1.913526     3.831202     0.444629
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H    −1.333096     5.281297     2.255652
H    −1.361889     3.955445     3.424476
H     0.851231     4.539324     1.386691
H     1.037301     4.275152     3.131353
H     1.432716     2.187972     1.487175
H     0.409751     1.918555     2.908156
H     0.335608    −2.783208     1.782387
H     1.315445    −2.759371     0.308032
H     1.005600    −5.125058     0.489106
H    −0.580962    −4.943920     1.255883
H     0.099796    −4.403382    −1.682376
H    −1.176134    −5.476228    −1.069088
H    −1.820856    −2.902744    −1.734738
H    −2.481807    −3.617181    −0.251056
H     2.258665    −1.150370     4.693259
H     0.795234    −0.579634     2.793128
H     4.716184    −1.321361     4.391632
H     0.475540     2.602524    −1.021676
H     1.734899     4.477191    −1.955923
H     4.215399     4.415099    −2.076172
H     5.709612    −0.895395     2.143664
H     5.419701     2.363252    −1.326117
H     0.115478    −1.440283    −2.183593
H     5.025594    −2.081513    −2.449686
H     1.074027    −2.833282    −3.952022
H     3.522445    −3.230534    −4.076770

LA−5e_LB−1
    42
xyz
N    −2.383417     4.224824     1.310054
H    −2.742773     4.150181     0.369810
H    −3.041280     3.991308     2.041697
N    −0.658677     5.541102     0.545796
H     0.050269     6.240877     0.705831
H    −0.439668     4.848668    −0.154950
N    −1.405602     5.772950     2.739940
H    −0.604357     6.374097     2.886280
C    −1.481085     5.193571     1.566917
F    −6.964200     5.957563     5.700111
F    −4.346331     2.749039     7.417035
F    −3.634012     7.030040     8.460782
F    −4.884639     5.250516     7.049285
C    −6.135878     6.108495     4.664838
C    −3.490790     2.874721     6.400405
C    −2.804776     7.146624     7.421817
F    −7.996179     6.864651     3.415769
F    −2.876198     0.621384     6.768913
F    −1.627462     8.771047     8.674000
C    −4.037926     5.369615     5.983771
C    −6.693650     6.589950     3.479283
C    −2.725276     1.752038     6.079530
C    −1.758777     8.063896     7.551657
C    −4.782196     5.819281     4.724698
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C    −3.333976     4.046052     5.677899
C    −2.941063     6.411825     6.255935
C    −5.888856     6.793114     2.373384
C    −1.799292     1.818350     5.054290
C    −0.857487     8.238318     6.516433
C    −3.950502     5.990689     3.600527
C    −2.421341     4.123138     4.608499
C    −2.034180     6.580157     5.192566
B    −2.384672     5.616883     3.927832
F    −6.413525     7.269316     1.242636
F    −1.051263     0.753654     4.760096
F     0.143126     9.111098     6.637689
C    −4.529040     6.499244     2.454262
C    −1.653947     3.006644     4.340271
C    −1.013859     7.489349     5.353304
F    −3.800477     6.752284     1.341750
F    −0.707975     3.013769     3.375491
F    −0.100028     7.693267     4.365227

LA−5e_LB−2
    67
xyz
C     2.405101    −3.083790    −2.262876
C     2.999848    −2.056551    −1.530588
C     2.211659    −1.146387    −0.844661
C     0.802766    −1.223122    −0.869665
C     0.252863    −2.266611    −1.592889
C     1.028986    −3.191275    −2.289619
B     0.116949     0.000196     0.000091
C     0.802621     1.365002    −0.624738
C     0.252543     2.513158    −1.166404
C     1.028514     3.578993    −1.618838
C     2.404644     3.502121    −1.539447
C     2.999552     2.354232    −1.016355
C     2.211530     1.304937    −0.571256
C     2.764874     0.000392    −0.000488
C     2.212061    −0.157523     1.414830
C     0.803200    −0.141165     1.494205
C     0.253737    −0.246109     2.759659
C     1.030285    −0.387160     3.908546
C     2.406365    −0.417520     3.801632
C     3.000651    −0.296670     2.545686
P    −1.885005     0.000047     0.000330
C    −2.585644    −0.161315    −1.678685
C    −1.839273     0.229549    −2.793860
C    −2.371066     0.102258    −4.072264
C    −3.650722    −0.417951    −4.250771
C    −4.392494    −0.824792    −3.145009
C    −3.860169    −0.704398    −1.864547
C    −2.585203    −1.373754     0.979410
C    −1.838637    −2.534963     1.197801
C    −2.370064    −3.578894     1.946869
C    −3.649609    −3.473880     2.486975
C    −4.391640    −2.312894     2.287067
```

```
C        -3.859681       -1.263750        1.542890
C        -2.586084        1.534600        0.700232
C        -3.861090        1.966108        0.323365
C        -4.394120        3.134861        0.859439
C        -3.652612        3.889693        1.764335
C        -2.372490        3.476025        2.125068
C        -1.839987        2.305636        1.595953
H        -0.830600       -2.626630        0.809459
H        -4.436507       -0.350940        1.427743
H        -1.777360       -4.473132        2.114027
H        -5.382098       -2.214392        2.721215
H        -4.061577       -4.289540        3.073751
H        -4.437481        1.408990       -0.409181
H        -0.831385        2.016736        1.869023
H        -5.384997        3.460430        0.557180
H        -1.780147        4.068971        2.815317
H        -4.065410        4.805474        2.176979
H        -0.831059        0.611356       -2.679505
H        -4.436675       -1.060771       -1.016099
H        -1.778532        0.404056       -4.930589
H        -5.382988       -1.250065       -3.276345
H        -4.062942       -0.518730       -5.250388
F         0.449316       -0.487047        5.104516
F        -1.075875       -0.192968        2.967520
F         3.161311       -0.552145        4.890892
F        -1.077195        2.665955       -1.316017
F         0.446965        4.664467       -2.130102
F         3.159060        4.513074       -1.967671
F         4.334680       -0.323558        2.511917
F         4.333601        2.339071       -0.976676
F         4.130798        0.000526       -0.000706
F        -1.076798       -2.473083       -1.650135
F         4.333888       -2.014419       -1.537255
F         0.447582       -4.177088       -2.973719
F         3.159646       -3.960126       -2.924121

LA-5e_LB-3
    73
xyz
  P         2.563742        0.000190        0.000159
  C         3.325661       -1.701037       -0.623525
  C         3.325076        1.391645       -1.161034
  C         3.324577        0.310939        1.785937
  C         3.541941       -1.874452       -2.163852
  H         3.259013       -1.035389       -2.786027
  H         4.597559       -2.080089       -2.364986
  H         2.971899       -2.733485       -2.523367
  C         2.356209       -2.812018       -0.175343
  H         2.740510       -3.774930       -0.531928
  H         2.250581       -2.883680        0.905458
  H         1.358918       -2.673616       -0.604670
  C         4.722115       -1.970927       -0.016392
  H         5.034378       -2.966147       -0.355552
  H         5.466322       -1.260262       -0.383635
```

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H	4.761112	−1.982453	1.067075
C	2.354621	1.559032	−2.346398
H	2.738754	2.348553	−3.002993
H	2.247934	0.658477	−2.948028
H	1.357772	1.862379	−2.011149
C	3.541477	2.812047	−0.540510
H	4.597549	3.088052	−0.615044
H	2.973757	3.553413	−1.106476
H	3.255633	2.931720	0.496327
C	4.721134	1.001779	−1.699831
H	4.759775	0.070696	−2.253890
H	5.033073	1.794755	−2.390398
H	5.465633	0.962434	−0.901253
C	4.720600	0.972477	1.716390
H	5.033226	1.175609	2.747883
H	5.464719	0.299814	1.283424
H	4.758767	1.916883	1.185326
C	2.354106	1.254108	2.523107
H	2.738133	1.428234	3.535143
H	2.247132	2.225306	2.043787
H	1.357412	0.811849	2.618173
C	3.541154	−0.936117	2.706557
H	2.970458	−0.818465	3.629948
H	3.258587	−1.894511	2.290884
H	4.596679	−1.007086	2.985673
F	−4.200228	2.445915	0.435897
F	−4.199525	−0.848281	−2.336522
F	−4.199254	−1.599904	1.903116
F	−3.973605	−0.000421	0.000387
C	−2.866929	2.505751	0.412095
C	−2.866193	−0.897477	−2.376167
C	−2.865878	−1.609672	1.965192
F	−3.081723	4.834382	0.771449
F	−3.080067	−1.750919	−4.572482
F	−3.078863	−3.085656	3.802111
C	−2.608644	−0.000327	0.000175
C	−2.305648	3.768578	0.589301
C	−2.304388	−1.374909	−3.558400
C	−2.303649	−2.395053	2.969344
C	−2.056335	1.396648	0.223870
C	−2.056008	−0.505142	−1.321452
C	−2.055909	−0.892140	1.098060
C	−0.934789	3.892261	0.564352
C	−0.933451	−1.456982	−3.653175
C	−0.932646	−2.435969	3.087205
C	−0.642673	1.484176	0.211550
C	−0.642337	−0.558287	−1.391297
C	−0.642215	−0.925517	1.178726
B	0.077635	0.000223	−0.000318
F	−0.358418	5.085779	0.717363
F	−0.356665	−1.920628	−4.763335
F	−0.355330	−3.165970	4.043206
C	−0.146916	2.758682	0.373554
C	−0.146006	−1.054650	−2.576049

```
C     −0.145555    −1.703912     2.200293
F      1.168691     3.000033     0.339990
F      1.169756    −1.203076    −2.768081
F      1.170276    −1.796055     2.424211
```

LA−5e_LB−4
```
  66
xyz
P      3.020958    −0.013339    −0.226616
N      4.160049     1.088173    −0.757754
N      3.732820    −1.441704    −0.661503
N      2.878866     0.157368     1.410026
C      4.794934     0.992799    −2.066513
H      4.488981     1.825052    −2.713352
H      4.528011     0.058087    −2.561878
H      5.886242     1.026151    −1.951499
C      4.397332     2.366592    −0.101649
H      4.053389     2.345009     0.931400
H      3.892328     3.189557    −0.621594
H      5.475957     2.564949    −0.093609
C      5.153692    −1.708086    −0.482643
H      5.656170    −0.853638    −0.025987
H      5.626342    −1.912570    −1.452414
H      5.298485    −2.586446     0.159293
C      2.993345    −2.559435    −1.237104
H      3.426289    −2.814163    −2.212987
H      1.949236    −2.290619    −1.379922
H      3.048812    −3.436584    −0.583125
C      2.116147     1.210256     2.071583
H      2.778916     1.809754     2.710189
H      1.330215     0.771396     2.696960
H      1.650029     1.871753     1.347507
C      3.704820    −0.614982     2.328560
H      4.565116    −0.028324     2.680711
H      4.058697    −1.533477     1.863071
H      3.097306    −0.900343     3.194339
N      1.560847     0.117107    −0.939212
C      1.646021     0.639193    −2.321160
H      2.195220     1.581543    −2.361378
H      0.637848     0.837226    −2.684786
H      2.108968    −0.083957    −2.999456
F     −4.686759    −0.921651    −1.143941
F     −3.272064    −0.977518     3.084216
F     −3.797631     2.802754     0.971384
F     −3.731321     0.243774     0.908884
C     −3.423430    −1.055729    −1.557702
C     −2.045287    −1.198137     2.604071
C     −2.528945     2.759579     0.556854
F     −4.272168    −2.298768    −3.384076
F     −1.705357    −2.650116     4.443818
F     −2.537200     5.126178     0.592099
C     −2.435992     0.191766     0.473755
C     −3.228200    −1.785622    −2.730993
C     −1.247290    −2.085634     3.325629
```

```
C    −1.890456     3.982635     0.364500
C    −2.337838    −0.523076    −0.881572
C    −1.561467    −0.607440     1.446614
C    −1.844462     1.578111     0.315713
C    −1.945830    −1.991521    −3.199029
C     0.004031    −2.410475     2.842092
C    −0.576478     3.999039    −0.061983
C    −1.021205    −0.675614    −1.369516
C    −0.237731    −0.828966     1.000257
C    −0.507699     1.558457    −0.119415
B     0.105817     0.028426    −0.372525
F    −1.743937    −2.714960    −4.303005
F     0.759019    −3.311774     3.479020
F     0.054496     5.163210    −0.241359
C    −0.867122    −1.444369    −2.506014
C     0.470018    −1.802081     1.678581
C     0.086504     2.796702    −0.294498
F     0.353286    −1.734863    −3.013019
F     1.650723    −2.276204     1.225306
F     1.381294     2.935185    −0.676108
```

LA−5e_LB−5
```
   68
xyz
P     2.014828     0.001214     0.000314
N     5.265020     0.000665    −0.001613
N     2.648161    −1.514547    −0.298487
N     2.647885     1.016953    −1.163489
N     2.649177     0.499849     1.462073
C     5.155781    −1.437142    −0.058051
H     5.952228    −1.902138     0.545918
H     5.327209    −1.749820    −1.094863
C     3.815583    −1.996149     0.435451
H     3.826927    −3.088782     0.358988
H     3.699633    −1.759355     1.498354
C     5.157082     0.670408     1.271683
H     5.952682     1.427063     1.370988
H     5.331052    −0.070861     2.060587
C     3.816723     1.376186     1.512362
H     3.829872     1.852451     2.498696
H     3.699880     2.181250     0.779209
C     5.155145     0.768333    −1.218327
H     5.951026     0.477406    −1.923556
H     5.326931     1.822565    −0.970929
C     3.814500     0.621301    −1.948391
H     3.826010     1.234561    −2.855921
H     3.697959    −0.417208    −2.275726
C     1.992525    −2.471888    −1.179013
H     0.968528    −2.165265    −1.394898
C     1.991705     0.220768     2.731646
H     2.525328    −0.542033     3.312899
C     1.990669     2.256563    −1.554970
H     1.934308     2.311354    −2.647498
H     1.930710     1.141326     3.322201
```

```
H     0.971365    -0.129819     2.574181
H     1.940770    -3.447652    -0.684042
H     2.520966    -2.583733    -2.134432
H     0.968522     2.292210    -1.177152
H     2.521118     3.141053    -1.179654
F    -4.237135    -0.078165    -2.512812
F    -4.235346    -2.141659     1.324520
F    -4.237623     2.215814     1.188407
F    -4.019205    -0.001342     0.000990
C    -2.903396    -0.112042    -2.552503
C    -2.901615    -2.157295     1.373506
C    -2.903880     2.266724     1.179495
F    -3.086476    -0.236027    -4.907385
F    -3.082970    -4.135329     2.657548
F    -3.087753     4.368766     2.248053
C    -2.652995    -0.000938     0.000796
C    -2.322718    -0.195522    -3.816922
C    -2.320062    -3.210259     2.077679
C    -2.323566     3.403926     1.738913
C    -2.103374    -0.068652    -1.421338
C    -2.102379    -1.198289     0.770568
C    -2.103634     1.265000     0.652518
C    -0.948499    -0.245424    -3.925665
C    -0.945934    -3.278319     2.175338
C    -0.949429     3.523128     1.750835
C    -0.693448    -0.098240    -1.501383
C    -0.692441    -1.251508     0.836741
C    -0.693811     1.349824     0.666589
B     0.006270     0.000561     0.000481
F    -0.374291    -0.339734    -5.126581
F    -0.370916    -4.271163     2.856872
F    -0.375625     4.610419     2.269895
C    -0.161308    -0.200205    -2.776060
C    -0.159575    -2.304481     1.561894
C    -0.161986     2.504742     1.215935
F     1.164927    -0.288350    -3.005261
F     1.166653    -2.458106     1.753139
F     1.164376     2.747170     1.255304
```

LA-5e_LB-6
```
   86
xyz
 C    -0.856925    -0.050451    -0.227919
 N    -3.022084     0.598717     0.223645
 C    -1.702167     1.012624     0.113426
 N    -3.075710    -0.726327    -0.279997
 C    -4.105590     1.405297    -0.269607
 C    -1.757115    -1.057163    -0.629230
 C    -3.856746    -1.601591     0.564740
 N    -1.428355     2.319803     0.289163
 C    -0.360250     3.048354    -0.414458
 C    -2.187133     3.200365     1.187893
 N    -1.541167    -2.182283    -1.312478
 C    -0.338917    -2.426681    -2.123913
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C    −2.578874    −3.182531    −1.599069
C    −3.309536    −2.116524     1.737335
C    −5.170852    −1.875642     0.204033
C    −4.086925    −2.941215     2.544645
C    −5.404316    −3.229728     2.187867
C    −5.947725    −2.692801     1.021911
C    −5.217210     1.599956     0.541041
C    −4.036682     1.968468    −1.542810
C    −6.276460     2.376500     0.074543
C    −6.210837     2.957034    −1.190162
C    −5.090735     2.753073    −1.998094
C    −1.215049     4.353420     1.418121
C    −0.553975     4.497978     0.044256
C    −0.449112    −3.906713    −2.458746
C    −1.955176    −4.081062    −2.672827
H    −2.285464    −1.874029     2.005544
H    −3.663421    −3.356823     3.453951
H    −6.008150    −3.873169     2.820974
H    −6.974611    −2.913004     0.745790
H    −5.569716    −1.450984    −0.712465
H    −5.238052     1.149800     1.528837
H    −7.147574     2.534134     0.703390
H    −7.032321     3.570111    −1.548948
H    −5.040989     3.203566    −2.984988
H    −3.159307     1.795293    −2.160605
H    −2.456227     2.658184     2.097700
H    −3.105406     3.565592     0.711310
H    −1.724107     5.262485     1.748811
H    −0.473827     4.078713     2.176237
H    −1.226449     5.028425    −0.639862
H     0.393801     5.040906     0.076135
H    −0.475178     2.928330    −1.495388
H     0.627108     2.680320    −0.130903
H     0.572026    −2.171815    −1.591922
H    −0.393372    −1.809496    −3.030186
H     0.144673    −4.175670    −3.335770
H    −0.105737    −4.508433    −1.609334
H    −2.233021    −3.725955    −3.671574
H    −2.290258    −5.116686    −2.577685
H    −3.496520    −2.692552    −1.941420
H    −2.811114    −3.745159    −0.688875
F     5.182708    −2.186904     0.570172
F     5.008337     1.160402    −2.329938
F     4.745782     2.021433     1.994718
F     4.794996     0.293592     0.092171
C     3.851983    −2.301946     0.620010
C     3.679662     1.033416    −2.393575
C     3.430817     1.786973     2.048227
F     4.183696    −4.535996     1.332249
F     3.806280     1.797438    −4.630040
F     3.384851     3.073788     4.036393
C     3.433317     0.177199     0.026094
C     3.350131    −3.538094     1.029947
C     3.071856     1.370304    −3.600723
```

```
C     2.740487     2.334929     3.129812
C     2.984924    -1.268229     0.304313
C     2.903377     0.589397    -1.333204
C     2.752837     1.027381     1.108254
C     1.985112    -3.713231     1.147205
C     1.698675     1.257357    -3.729073
C     1.393287     2.066459     3.283441
C     1.583382    -1.449857     0.342745
C     1.508098     0.471381    -1.432569
C     1.356334     0.843144     1.182844
B     0.756945    -0.066295    -0.066628
F     1.492730    -4.881396     1.571983
F     1.109008     1.578877    -4.885463
F     0.736278     2.534997     4.350410
C     1.129452    -2.663733     0.818912
C     0.941403     0.811483    -2.649845
C     0.729012     1.303943     2.324849
F    -0.188543    -2.908528     0.996191
F    -0.393582     0.741328    -2.873355
F    -0.559799     1.009253     2.607641

LA–5f_LB–1
    41
xyz
C    -1.018153     7.505726     5.346765
C    -0.816670     8.272827     6.497041
C    -1.674119     8.143090     7.582586
C    -2.730244     7.239888     7.501137
C    -2.891742     6.499551     6.339837
C    -2.051649     6.598073     5.222256
F    -3.559719     7.102552     8.528369
F    -1.489595     8.865293     8.673642
S    -4.251297     5.338658     6.238009
C    -3.326844     3.914026     5.695230
C    -3.447679     2.733381     6.412597
C    -2.646362     1.651821     6.061382
C    -1.736059     1.805041     5.023550
C    -1.638459     3.018294     4.333599
C    -2.444343     4.107904     4.624274
F    -4.299344     2.623478     7.425087
F    -2.735795     0.506182     6.713462
F    -0.952100     0.795363     4.691695
F     0.189753     9.124264     6.556669
B    -2.432498     5.623358     3.955935
C    -4.004736     6.022412     3.619878
C    -4.917986     5.867291     4.671132
C    -6.264293     6.191899     4.599352
C    -6.765455     6.709261     3.409201
C    -5.892246     6.906674     2.347230
C    -4.537941     6.576141     2.466483
F    -7.071588     6.028397     5.640552
F    -8.043657     7.023982     3.295867
F    -6.347114     7.417470     1.217510
F    -3.776382     6.842753     1.397006
```

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F    -0.701415     3.071291     3.377515
F    -0.139647     7.694919     4.341031
N    -1.473250     5.782916     2.768921
C    -1.495579     5.149703     1.605939
N    -0.569563     5.408142     0.668647
N    -2.438385     4.238859     1.332171
H    -2.460167     3.742182     0.455425
H    -3.154309     4.016368     2.005983
H     0.167029     6.077087     0.833235
H    -0.569572     4.941602    -0.225299
H    -0.726362     6.456750     2.873562
```

LA-5f_LB-2
```
    66
xyz
C    -1.788610     0.732787     2.715150
C    -2.530536     0.722103     1.530000
C    -3.804228     1.299171     1.514604
C    -4.338778     1.848752     2.676324
C    -3.601257     1.841892     3.856976
C    -2.322316     1.289682     3.871722
P    -1.847993     0.000739     0.000154
C    -2.529719    -1.685088    -0.140841
C    -1.786280    -2.716418    -0.723056
C    -2.319049    -3.996843    -0.819553
C    -3.598478    -4.260864    -0.335505
C    -4.337512    -3.242192     0.259565
C    -3.803960    -1.960910     0.364915
B     0.164880     0.000382     0.000851
C     0.835491    -1.098490     1.058046
C     2.240222    -1.147516     1.054012
C     3.013221    -2.002616     1.824530
C     2.380941    -2.894207     2.682447
C     0.996174    -2.875365     2.741045
C     0.254133    -1.990387     1.950029
S     3.096860    -0.000795     0.000714
F    -1.065766    -2.048509     2.136769
F     0.367338    -3.698987     3.559650
F     3.080520    -3.728156     3.431227
F     4.340151    -1.980357     1.756526
C     0.835763    -0.366609    -1.479218
C     2.240478    -0.339138    -1.519312
C     3.013701    -0.579782    -2.644743
C     2.381641    -0.877684    -3.845814
C     0.996851    -0.937794    -3.859035
C     0.254623    -0.694228    -2.697433
F     3.081461    -1.110170    -4.942048
F     4.340629    -0.532338    -2.591138
F    -1.065287    -0.827023    -2.841146
F     0.368263    -1.235946    -4.981484
C     0.836474     1.465179     0.423458
C     0.256217     2.684394     0.749123
C     0.999270     3.811550     1.119219
C     2.384015     3.769143     1.164621
```

```
C      3.015185    2.579698    0.821857
C      2.241254    1.485272    0.467401
F     −1.063452    2.876650    0.705513
F      0.371411    4.933046    1.422442
F      3.084575    4.834252    1.511454
F      4.342064    2.508639    0.836094
C     −2.527480    0.965766   −1.390450
C     −1.783399    1.986537   −1.990196
C     −2.314133    2.710399   −3.051770
C     −3.592151    2.422407   −3.525695
C     −4.331831    1.396907   −2.943278
C     −3.800319    0.664977   −1.885368
H     −0.779612   −2.542314   −1.086979
H     −4.380754   −1.188619    0.864597
H     −1.731561   −4.790498   −1.270742
H     −5.327974   −3.444161    0.655024
H     −4.013168   −5.261150   −0.411926
H     −4.379874    1.346400    0.595258
H     −0.782476    0.329438    2.747715
H     −5.328876    2.292985    2.652327
H     −1.735939    1.295080    4.785364
H     −4.016658    2.276088    4.760989
H     −0.778000    2.215838   −1.654434
H     −4.377446   −0.154518   −1.468023
H     −1.726270    3.498801   −3.511607
H     −5.321254    1.154890   −3.318363
H     −4.005252    2.988674   −4.354583

LA−5f_LB−3
   72
xyz
C     −0.156251    0.205576   −2.786930
C     −0.909341    0.341321   −3.959185
C     −2.290021    0.393928   −3.910985
C     −2.886142    0.295408   −2.660962
C     −2.090564    0.167789   −1.532217
C     −0.680437    0.128833   −1.511621
F     −4.211660    0.320614   −2.560510
F     −3.013127    0.520730   −5.008005
S     −2.951094   −0.000523    0.000657
C     −2.090284    1.242705    0.912613
C     −2.885445    2.156303    1.588186
C     −2.288952    3.190034    2.297540
C     −0.908356    3.259092    2.273905
C     −0.155799    2.312032    1.569376
C     −0.680251    1.244940    0.867003
F     −4.210949    2.056186    1.561319
F     −3.011703    4.076361    2.956687
F     −0.283758    4.230105    2.916806
F     −0.285093    0.414184   −5.121654
B      0.049301    0.000199   −0.000178
C     −0.679912   −1.373423    0.644162
C     −2.089932   −1.411756    0.621122
C     −2.884668   −2.453683    1.075134
```

```
C      −2.287578     −3.585126      1.614479
C      −0.906869     −3.599597      1.683735
C      −0.154810     −2.515913      1.215114
F      −4.210261     −2.380195      1.003511
F      −3.009824     −4.599160      2.053243
F      −0.281673     −4.642363      2.201534
F       1.153816     −2.653684      1.377491
F       1.152567      2.523955      1.605317
F       1.152246      0.134100     −2.988666
P       2.505191     −0.000029     −0.000178
C       3.265165     −1.287388     −1.289992
C       3.473605     −0.803054     −2.764166
C       3.264718      1.760903     −0.469623
C       4.667827      1.612370     −1.105770
C       3.264219     −0.473236      1.759884
C       4.667738      0.151064      1.949532
C       3.476005      2.794163      0.687736
C       2.318368      2.421568     −1.489706
C       2.317695      0.081303      2.841198
C       3.474259     −1.992073      2.076974
C       4.669308     −1.761589     −0.843701
C       2.320926     −2.502856     −1.350470
H       3.266749      2.446777      1.691222
H       4.516213      3.131047      0.681744
H       2.854180      3.675520      0.523769
H       2.694047      3.427384     −1.707014
H       2.263147      1.889704     −2.436935
H       1.303009      2.530935     −1.092436
H       4.977641      2.612962     −1.428429
H       5.408062      1.268703     −0.380921
H       4.718980      0.974016     −1.980111
H       2.692267     −0.233311      3.821370
H       2.263424      1.167672      2.853540
H       1.301984     −0.316292      2.736554
H       4.513230     −2.155061      2.376183
H       2.848793     −2.291081      2.919403
H       3.268686     −2.687252      1.273235
H       4.719806      1.227366      1.834176
H       4.977106     −0.070044      2.977466
H       5.407902     −0.305201      1.289680
H       4.979100     −2.542732     −1.547340
H       5.408844     −0.961576     −0.911063
H       4.721748     −2.197342      0.147264
H       2.696238     −3.192702     −2.114208
H       2.268917     −3.058046     −0.416559
H       1.304375     −2.215283     −1.641402
H       2.846588     −1.382294     −3.443537
H       3.269562      0.240875     −2.964300
H       4.511997     −0.982282     −3.056128
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LA−5f_LB−4
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    65
xyz
C       0.201837      2.811662     −0.268150
```

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C    -0.354665     4.066732    -0.008743
C    -1.647967     4.186611     0.480694
C    -2.369410     3.023244     0.706888
C    -1.770854     1.802096     0.429440
C    -0.477131     1.615599    -0.066947
F    -3.609919     3.091642     1.178698
F    -2.171479     5.375104     0.727681
S    -2.713537     0.332133     0.704827
C    -1.518546    -0.630021     1.614300
C    -1.973234    -1.271148     2.758209
C    -1.168207    -2.228518     3.362286
C     0.027807    -2.557837     2.741975
C     0.433521    -1.904012     1.574908
C    -0.269670    -0.853486     1.006747
F    -3.172511    -1.003789     3.265961
F    -1.554962    -2.848989     4.464401
F     0.786448    -3.516083     3.251257
F     0.363713     5.157147    -0.222705
B     0.043465     0.038771    -0.365039
C    -1.158570    -0.613107    -1.341396
C    -2.477464    -0.449228    -0.885194
C    -3.605592    -0.945859    -1.520723
C    -3.453077    -1.672684    -2.695478
C    -2.167945    -1.900649    -3.164575
C    -1.057070    -1.389650    -2.484485
F    -4.821646    -0.751947    -1.019061
F    -4.504351    -2.157483    -3.335192
F    -1.992138    -2.617664    -4.261042
F     0.130492    -1.723683    -3.008992
F     1.534189    -2.408180     1.005032
F     1.473293     2.853833    -0.700728
N     1.463379     0.059593    -0.975327
C     1.533659     0.577543    -2.362600
P     2.958751    -0.095921    -0.299016
N     2.822962    -0.014160     1.347776
C     3.657127    -0.850763     2.208136
N     4.073022     1.035127    -0.789099
C     4.447449     2.211677    -0.011458
N     3.637416    -1.501823    -0.823175
C     2.896079    -2.591434    -1.450955
C     4.686290     1.010791    -2.116080
C     5.068877    -1.770585    -0.695103
C     2.156892     1.064037     2.071639
H     4.421778     1.912170    -2.681622
H     4.359848     0.137819    -2.682875
H     5.777797     0.970604    -2.017271
H     4.175760     2.094567     1.036063
H     3.976810     3.120944    -0.401981
H     5.535269     2.332729    -0.060672
H     5.577690    -0.950026    -0.186980
H     5.518995    -1.901312    -1.686475
H     5.227239    -2.690836    -0.120828
H     3.314727    -2.785031    -2.445917
H     1.847329    -2.326822    -1.558660
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H    2.974223   −3.504883   −0.851930
H    2.867937    1.572976    2.734276
H    1.342406    0.662531    2.686735
H    1.746683    1.803558    1.388949
H    4.551978   −0.310908    2.544900
H    3.955935   −1.763819    1.695403
H    3.074200   −1.140908    3.088981
H    2.129626    1.488666   −2.421425
H    0.529863    0.830637   −2.705298
H    1.943496   −0.168236   −3.049187

LA−5f_LB−5
    67
xyz
C   −0.169055   −2.743137    0.582639
C   −0.926793   −3.904692    0.776825
C   −2.309913   −3.877475    0.712387
C   −2.922545   −2.656772    0.462138
C   −2.133340   −1.532682    0.270702
C   −0.726900   −1.500395    0.302641
F   −4.248429   −2.582053    0.411740
F   −3.022678   −4.974022    0.896640
S   −2.986350   −0.000646    0.000941
C   −2.134350    0.531648   −1.461356
C   −2.924175    0.927776   −2.530202
C   −2.312247    1.321492   −3.712810
C   −0.929128    1.279714   −3.769326
C   −0.170767    0.867260   −2.666707
C   −0.727943    0.488061   −1.450230
F   −4.250014    0.933863   −2.439613
F   −3.025673    1.710064   −4.754186
F   −0.311345    1.631042   −4.883589
F   −0.308388   −5.044981    1.029799
B   −0.038607    0.000058   −0.000145
C   −0.727155    1.012012    1.147907
C   −2.133517    0.999632    1.192442
C   −2.922734    1.727502    2.070230
C   −2.310098    2.555430    3.001491
C   −0.927001    2.625648    2.992147
C   −0.169320    1.876653    2.083351
F   −4.248603    1.645849    2.031318
F   −3.022837    3.263428    3.858913
F   −0.308620    3.415789    3.852363
F    1.146781    2.086970    2.177767
F    1.145317    0.845808   −2.896364
F    1.147150   −2.930505    0.716557
P    1.993306    0.000341   −0.000318
N    2.592651   −1.312486   −0.828495
C    1.961461   −1.848948   −2.027635
N    2.592660    1.373767   −0.723500
C    1.961432    2.680521   −0.588248
N    2.592876   −0.060359    1.550569
C    1.961403   −0.830298    2.614842
C    3.769646    1.308133   −1.595996
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```
C      5.097712     1.165964    -0.844959
N      5.145894    -0.000210    -0.000579
C      5.097909     0.147902     1.431532
C      3.770078     0.727439     1.930551
C      5.097534    -1.314550    -0.588378
C      3.769437    -2.035794    -0.335692
H      5.908539     1.145455    -1.590018
H      5.269388     2.050753    -0.221624
H      3.778720     2.216541    -2.206558
H      3.658628     0.467197    -2.287997
H      5.908527    -1.949556    -0.198500
H      5.268727    -1.216969    -1.666358
H      3.778079    -3.018661    -0.817345
H      3.658646    -2.214989     0.738524
H      5.908964     0.803096     1.786288
H      5.269358    -0.834413     1.886023
H      3.779154     0.800853     3.022625
H      3.659469     1.747696     1.549507
H      0.929351     2.584346    -0.247184
H      2.495180    -1.564240    -2.942384
H      1.927783    -0.227741     3.528204
H      1.930397    -2.941361    -1.963818
H      0.930754    -1.502274    -2.117141
H      1.933871     3.172965    -1.565516
H      2.492891     3.329121     0.118474
H      0.931713    -1.083847     2.357857
H      2.496610    -1.763558     2.827607


LA−5f_LB−6
    85
xyz
 C      0.723313     1.342823     2.289256
 C      1.331563     2.147444     3.256586
 C      2.674948     2.486202     3.161265
 C      3.415417     1.957811     2.111159
 C      2.767342     1.182928     1.159971
 C      1.392916     0.901566     1.157405
 F      4.726477     2.175948     2.051137
 F      3.246791     3.246923     4.082516
 S      3.777932     0.233754     0.031597
 C      2.957147     0.591944    -1.494388
 C      3.719188     0.996818    -2.582392
 C      3.074064     1.265135    -3.780468
 C      1.693322     1.114119    -3.835069
 C      0.969661     0.705199    -2.713350
 C      1.570176     0.428549    -1.489046
 F      5.039713     1.126677    -2.493262
 F      3.752138     1.653187    -4.848895
 F      1.059704     1.365763    -4.970521
 F      0.623079     2.585743     4.286629
 B      0.826568    -0.060692    -0.083817
 C      1.640856    -1.437712     0.408283
 C      3.044078    -1.360240     0.391682
 C      3.896144    -2.377082     0.797736
```

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C      3.351263    −3.562730     1.275731
C      1.970110    −3.662770     1.369985
C      1.148089    −2.608685     0.961982
F      5.217667    −2.228762     0.759207
F      4.130018    −4.560829     1.663829
F      1.428586    −4.768272     1.857576
F     −0.164632    −2.798916     1.145873
F     −0.354837     0.605988    −2.906340
F     −0.538662     0.982743     2.557276
C     −0.779532    −0.061283    −0.251752
C     −1.625178     1.013969     0.065772
N     −2.930450     0.597991     0.175263
N     −2.984862    −0.730144    −0.300213
C     −1.678487    −1.088361    −0.622597
C     −4.057137     1.395954    −0.226849
C     −5.097322     1.590548     0.673269
C     −6.193357     2.360508     0.289197
C     −6.234771     2.928583    −0.982359
C     −5.186699     2.720465    −1.880787
C     −4.094958     1.943971    −1.507285
N     −1.330725     2.323323     0.230125
C     −0.309854     3.038148    −0.551446
C     −0.526543     4.507436    −0.170988
C     −1.141827     4.427254     1.228840
C     −2.091452     3.241436     1.094001
C     −3.867888    −1.576475     0.470370
C     −3.436552    −2.104409     1.684445
C     −4.307057    −2.896140     2.427312
C     −5.600159    −3.137074     1.962780
C     −6.026963    −2.584952     0.756061
C     −5.157659    −1.799389     0.003382
N     −1.455102    −2.245596    −1.253660
C     −0.252752    −2.517236    −2.055300
C     −0.366211    −4.005288    −2.352569
C     −1.869756    −4.173878    −2.582744
C     −2.505130    −3.237943    −1.548541
H     −2.431028    −1.894974     2.037546
H     −3.977675    −3.321732     3.370131
H     −6.277522    −3.754093     2.545136
H     −7.035797    −2.766773     0.398981
H     −5.468364    −1.361281    −0.940412
H     −5.038526     1.145396     1.661783
H     −7.011091     2.519722     0.985061
H     −7.086394     3.533944    −1.277214
H     −5.224160     3.159781    −2.872914
H     −3.272761     1.764893    −2.195394
H     −2.330341     2.749417     2.040090
H     −3.026426     3.560597     0.620298
H     −1.663520     5.341396     1.521039
H     −0.371427     4.220309     1.980307
H     −1.234589     4.976896    −0.862469
H      0.404465     5.078368    −0.203519
H     −0.454790     2.856460    −1.620386
H      0.699830     2.714983    −0.281456
```

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H     0.660531    −2.255169    −1.529358
H    −0.298829    −1.928346    −2.980895
H     0.236745    −4.301558    −3.214090
H    −0.039133    −4.588407    −1.483678
H    −2.129652    −3.851056    −3.596554
H    −2.212602    −5.203390    −2.460386
H    −3.400235    −2.739550    −1.933038
H    −2.777019    −3.770158    −0.632146
```

LA−8f_LB−1
```
    22
xyz
N    −3.639766     0.939370     0.712604
H    −4.532906     1.414105     0.660357
H    −3.664308    −0.068868     0.687477
N    −1.361532     0.923155     0.424308
H    −0.517356     1.316331     0.037544
H    −1.253087     0.245811     1.163591
N    −2.582466     2.773414    −0.265000
H    −1.685427     3.243237    −0.316216
C    −2.541685     1.574293     0.277384
F    −5.752980     2.045608    −0.910587
F    −3.720879     5.266211     1.021792
F    −1.879326     5.177779    −1.298249
B    −3.762446     3.608914    −0.847815
C    −3.035488     4.682193    −1.856275
C    −4.522626     4.377063     0.384114
C    −4.812779     2.670662    −1.699410
F    −4.908706     3.486615     1.362153
F    −5.518426     3.355352    −2.616030
F    −2.636689     4.118922    −3.026617
F    −3.782060     5.751825    −2.176061
F    −5.639302     5.043306     0.035364
F    −4.192119     1.657531    −2.362769
```

LA−8f_LB−2
```
    47
xyz
P    −0.175633    −1.045082     1.222555
C     0.215577     0.735241     1.082014
C    −0.702307     1.648789     1.613434
C     1.347528     1.206728     0.414414
C    −0.472302     3.014730     1.501036
H    −1.603416     1.302128     2.107300
C     1.572505     2.577062     0.303807
H     2.055419     0.518582    −0.033158
C     0.668397     3.482178     0.851211
H    −1.187819     3.713365     1.923601
H     2.457769     2.932820    −0.214727
H     0.847941     4.549973     0.766871
C     1.026564    −1.966058     0.202011
C     0.573983    −2.782254    −0.839626
C     2.398635    −1.895688     0.472707
C     1.481809    −3.510166    −1.603315
```

```
H      −0.485949     −2.865404     −1.054874
C       3.300901     −2.621243     −0.297424
H       2.773503     −1.283855      1.284636
C       2.845415     −3.429763     −1.336138
H       1.117308     −4.144847     −2.405326
H       4.361811     −2.559365     −0.075261
H       3.551943     −4.000517     −1.931595
C      −1.762164     −1.182226      0.331811
C      −2.768272     −2.070191      0.714421
C      −1.928028     −0.404514     −0.823134
C      −3.928863     −2.177338     −0.049599
H      −2.667641     −2.673053      1.606300
C      −3.086024     −0.518273     −1.582671
H      −1.154151      0.292657     −1.131203
C      −4.089756     −1.406011     −1.196092
H      −4.708428     −2.865774      0.261854
H      −3.205319      0.089694     −2.474411
H      −4.996947     −1.491589     −1.787185
F      −0.004042     −3.922755      4.271096
F      −1.521305     −1.396026      5.221949
F       1.382834     −1.475970      5.092525
B      −0.168558     −1.695914      3.149814
C       1.352795     −1.499893      3.745805
C      −1.216635     −0.808574      4.047649
C      −0.568098     −3.293234      3.222201
F      −2.413157     −0.592235      3.418680
F      −1.907812     −3.520215      3.345569
F       2.210965     −2.484017      3.369930
F       1.944807     −0.335354      3.340181
F      −0.748576      0.428007      4.356788
F      −0.191937     −3.991626      2.113318

LA−8f_LB−3
    53
xyz
P      −1.003878      0.000070     −0.000241
C      −1.707042      1.143187     −1.401544
C      −1.707988     −1.784600     −0.289416
C      −1.708026      0.642075      1.690022
C      −1.548099      0.481170     −2.784908
H      −2.217657     −0.368416     −2.927949
H      −1.818816      1.229936     −3.538297
H      −0.528337      0.166165     −2.997407
C      −0.963090      2.490908     −1.470060
H      −1.448997      3.086479     −2.252463
H      −1.015762      3.063474     −0.546377
H       0.081528      2.376631     −1.744947
C      −3.203002      1.476898     −1.223465
H      −3.520236      2.017233     −2.123268
H      −3.848029      0.604127     −1.132859
H      −3.388111      2.141060     −0.378038
C      −0.964288     −2.518801     −1.421842
H      −1.452400     −3.492883     −1.547828
H      −1.013962     −2.004487     −2.379244
```

```
H      0.079440   −2.702471   −1.183709
C     −1.549339   −2.651438    0.975807
H     −2.220159   −2.351436    1.782366
H     −1.818414   −3.678612    0.703724
H     −0.530016   −2.676601    1.356012
C     −3.203998   −1.797152   −0.667375
H     −3.389476   −1.398831   −1.665948
H     −3.521476   −2.846526   −0.683560
H     −3.848697   −1.280996    0.042484
C     −3.204101    0.321472    1.890154
H     −3.520868    0.830716    2.808065
H     −3.849147    0.679705    1.089146
H     −3.389753   −0.742679    2.042684
C     −0.964399    0.027809    2.891738
H     −1.450802    0.407463    3.798511
H     −1.016812   −1.058374    2.925786
H      0.080099    0.323314    2.930732
C     −1.548800    2.171045    1.808112
H     −0.529165    2.512365    1.640771
H     −2.218712    2.719615    1.144237
H     −1.818838    2.449382    2.833372
F      3.104738   −1.107453    1.093116
F      3.105206    1.499486    0.413062
F      1.731487    1.111424   −2.207756
B      1.149885    0.000116    0.000297
C      1.797211   −0.068559   −1.529479
C      1.797043    1.359261    0.705919
C      1.796776   −1.290927    0.824274
F      1.730264    1.356260    2.066932
F      1.227486   −1.556386    2.031613
F      3.105176   −0.393288   −1.504056
F      1.228503   −0.982399   −2.362347
F      1.228864    2.537763    0.331008
F      1.730406   −2.467750    0.140486
```

LA−8f_LB−4
```
   46
xyz
 P     −1.649382    1.479409    0.654327
 N     −3.183837    1.112902    0.092855
 N     −0.710512    0.305327   −0.034170
 N     −1.227927    2.943986    0.040529
 C     −3.698636   −0.249356    0.163226
 H     −4.474372   −0.350268    0.933658
 H     −2.897066   −0.953571    0.396897
 H     −4.131186   −0.526606   −0.805976
 C     −4.211200    2.120794   −0.122178
 H     −3.770440    3.049597   −0.483523
 H     −4.792806    2.331119    0.787554
 H     −4.899857    1.757058   −0.892435
 C     −0.839360    0.009258   −1.456926
 H     −1.408063    0.784831   −1.972734
 H     −1.356612   −0.949129   −1.604558
 H      0.154982   −0.059686   −1.913607
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129

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C    -0.018724    -0.736888     0.716803
H    -0.068136    -0.545869     1.784932
H     1.034114    -0.778001     0.420796
H    -0.485211    -1.710365     0.508011
C    -1.771117     4.184427     0.588318
H    -2.453926     3.979978     1.414881
H    -2.310078     4.739154    -0.191124
H    -0.958204     4.804542     0.974174
C    -0.255763     3.132951    -1.027344
H    -0.747580     3.300375    -1.995265
H     0.414110     2.276145    -1.098603
H     0.357268     4.006367    -0.787273
N    -1.595865     1.496010     2.288727
C    -2.758647     0.849484     2.946788
H    -3.698077     1.191826     2.509114
H    -2.779526     1.131638     3.994426
H    -2.703159    -0.243045     2.891662
F     0.964659     0.907857     5.078292
F    -0.467421     3.548185     5.283609
F     1.854958     2.857473     3.517893
B    -0.474420     1.997514     3.282016
C     1.008030     2.315408     2.617437
C    -0.982200     3.381489     4.045877
C    -0.220749     0.822954     4.443929
F    -2.341373     3.443706     4.198872
F    -1.157036     0.809890     5.436178
F     1.634255     1.198347     2.140523
F     1.017071     3.184503     1.566855
F    -0.665326     4.522594     3.367447
F    -0.258514    -0.446026     3.919471
```

LA-8f_LB-5
```
    48
xyz
 P    11.446336    11.125325     5.109019
 N     8.370458    11.680673     4.358198
 N    10.440189    11.008626     6.431671
 N    11.214250    12.647544     4.473126
 N    10.865770    10.048354     3.978390
 C     8.052259    11.219551     5.687656
 H     7.116056    10.637830     5.679287
 H     7.863743    12.100737     6.312956
 C     9.140752    10.350664     6.338864
 H     8.839050    10.073589     7.355879
 H     9.236506     9.414677     5.783020
 C     8.546985    10.722946     3.293790
 H     7.989653    11.037917     2.396507
 H     8.101688     9.774400     3.617812
 C    10.009749    10.489691     2.881777
 H    10.059694     9.725191     2.097455
 H    10.411627    11.405551     2.441443
 C     8.758261    13.055078     4.153264
 H     7.963038    13.734970     4.500117
 H     8.856720    13.219157     3.073270
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130
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C     10.064266    13.460626     4.855922
H     10.306452    14.503965     4.621642
H      9.920978    13.415785     5.938366
C     10.704103    11.713673     7.682428
H     11.464925    12.482591     7.549438
C     11.010819     8.603161     4.125164
H     11.303684     8.336692     5.140559
C     12.018926    13.168521     3.372173
H     12.584077    12.373745     2.885605
H     10.047653     8.118057     3.925122
H     11.762883     8.208701     3.434272
H     11.043310    11.023641     8.461745
H      9.788273    12.215067     8.018457
H     12.724372    13.928719     3.722894
H     11.359079    13.610466     2.615637
F     14.685540     9.311392     7.147395
F     15.346614    12.058749     6.470643
F     15.470236     9.990323     4.433062
B     13.392790    10.773961     5.584023
C     14.319090    10.661346     4.222667
C     13.999996    11.993415     6.515755
C     13.547212     9.362466     6.425367
F     13.685610    11.876314     7.836134
F     12.537454     9.133877     7.316994
F     13.705145    10.018865     3.184764
F     14.690245    11.870489     3.716503
F     13.560858    13.236967     6.158358
F     13.570633     8.256184     5.630642

LA−8f_LB−6
    66
xyz
C      0.702743    −0.007929    −0.159583
N     −1.468312    −0.586576     0.199691
C     −0.239827    −1.067785    −0.129663
N     −1.384028     0.783856     0.380087
C     −2.695512    −1.280859     0.366348
C     −0.084248     1.135852     0.058471
C     −2.515599     1.551677    −0.062768
N     −0.100293    −2.397352    −0.379414
C     −0.478690    −3.492738     0.517665
C      0.396681    −2.869477    −1.677562
N      0.205827     2.458397     0.002564
C      0.861438     3.094745    −1.151778
C     −0.265852     3.434138     0.988254
C     −2.625800     1.882436    −1.411128
C     −3.476444     1.955976     0.855752
C     −3.714218     2.633898    −1.841894
C     −4.686674     3.040082    −0.928222
C     −4.569582     2.698940     0.417569
C     −3.260178    −1.923069    −0.731719
C     −3.302802    −1.324749     1.618708
C     −4.446055    −2.632309    −0.566967
C     −5.068427    −2.675479     0.679687
```

```
C   −4.500172   −2.016799    1.769384
C    0.488165   −4.384795   −1.487656
C   −0.584883   −4.683649   −0.433442
C    0.612150    4.585721   −0.904257
C    0.536415    4.681430    0.623037
H   −1.859313    1.555587   −2.108627
H   −3.804326    2.900629   −2.890495
H   −5.536202    3.625609   −1.266724
H   −5.324520    3.017654    1.129643
H   −3.356239    1.699301    1.903227
H   −2.764151   −1.870147   −1.695790
H   −4.889370   −3.143184   −1.416216
H   −5.997248   −3.224170    0.802683
H   −4.981317   −2.054861    2.741899
H   −2.826845   −0.833136    2.461918
H    1.353192   −2.417420   −1.936010
H   −0.333540   −2.612106   −2.461974
H    0.328958   −4.924048   −2.425434
H    1.477456   −4.649046   −1.103305
H   −1.580346   −4.701663   −0.895013
H   −0.428337   −5.636266    0.079684
H   −1.416650   −3.296022    1.043966
H    0.310613   −3.643222    1.264033
H    0.412144    2.738384   −2.085567
H    1.924416    2.869043   −1.177378
H    1.402681    5.205041   −1.335712
H   −0.344096    4.893550   −1.345279
H    1.538624    4.621027    1.058242
H    0.055269    5.598553    0.974104
H   −0.064059    3.064864    1.997937
H   −1.342009    3.634914    0.892011
F    3.008685    2.292557    0.600563
F    1.932789   −1.784528    1.938571
F    2.846848    1.046165   −2.087459
B    2.331671   −0.127275    0.088371
C    3.216004   −0.002841   −1.292497
C    2.719198   −1.562238    0.836676
C    2.807723    1.062729    1.163171
F    3.992895   −1.635999    1.280455
F    1.880836    1.272758    2.151904
F    4.545531    0.152061   −1.087061
F    3.101710   −1.093479   −2.110057
F    2.581711   −2.685977    0.074328
F    3.960238    0.815530    1.820791
```