

Periodic Trends in Trivalent Actinide Halides, Phosphates, and Arsenates

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1. Bond lengths and bond angles obtained from the optimized geometries

Table S1. An-X bond lengths obtained from optimized geometries using scalar ZORA relativistic method (Å)

Atom	F	Cl	Br	I	At	AsO₄	PO₄
Ac	2.19	2.67	2.83	3.05	3.14	2.28	2.27
Th	2.10	2.56	2.71	2.93	3.02	-	2.19
Pa	2.06	2.52	2.69	2.91	3.00	-	2.16
U	2.06	2.51	2.68	2.90	2.99	2.17	2.16
Np	2.06	2.51	2.68	2.89	2.99	2.16	2.16
Pu	2.06	2.51	2.67	2.89	2.99	2.16	2.16
Am	2.07	2.52	2.68	2.92	3.02	2.17	2.18
Cm	2.06	2.49	2.64	2.87	2.96	2.16	2.16
Bk	2.05	2.47	2.63	2.86	2.96	2.15	2.15
Cf	2.05	2.46	2.63	2.88	2.97	2.16	2.15
Es	2.05	2.47	2.63	2.88	2.98	2.16	2.17
Fm	2.04	2.49	2.65	2.91	3.01	2.17	2.19
Md	2.07	2.51	2.68	2.92	3.02	2.23	2.31
No	-	2.55	2.72	2.95	3.05	2.29	2.31
Lr	2.02	2.43	2.59	2.81	2.91	2.12	2.11

Table S2. Average of An-X bond lengths obtained from optimized geometries using spin-orbit ZORA relativistic method (Å)

Atom	F	Cl	Br	I	At	AsO₄	PO₄
Ac	2.19	2.66	2.83	3.05	3.17	2.28	2.27
Th	2.10	2.56	2.71	2.94	3.05		2.18
Pa	2.06	2.52	2.69	2.91	3.03		2.17
U	2.06	2.51	2.68	2.90	3.02	2.17	2.16

Np	2.06	2.51	2.67	2.89	3.02	2.163	2.16
Pu	2.07	2.50	2.66	2.89	3.01	2.16	2.16
Am	2.07	2.51	2.67	2.91	3.04	2.17	2.18
Cm	2.06	2.48	2.64	2.86	2.98	2.18	2.15
Bk	2.04	2.47	2.63	2.86	2.98	2.14	2.14
Cf	2.04	2.47	2.64	2.87	3.01	2.15	2.14
Es	2.05	2.47	2.64	2.87	3.02	2.16	2.15
Fm	2.04	2.48	2.64	2.90	3.03	2.17	2.16
Md	2.05	2.50	2.67	2.91	3.04	2.20	2.19
No		2.53	2.69	2.94	3.08	2.26	2.23
Lr	2.02	2.43	2.58	2.80	2.92	2.12	2.10

Table S3. Average of X-An-X bond angles obtained from optimized geometries (in degrees)

	F-An-F	Cl-An-Cl	Br-An-Br	I-An-I	At-An-At	O-An-O (in AnPO₄)	O-An-O (in AnAsO₄)
Ac	112.9	112.9	113.7	116.4	114.1	95.9	69.4
Th	119.9	119.8	120.0	120.0	119.9	66.4	-
Pa	106.4	111.7	114.0	115.7	115.6	67.5	-
U	102.7	106.1	108.6	109.9	108.9	67.6	72.5
Np	102.2	106.7	108.4	107.3	107.0	67.7	72.5
Pu	106.0	110.0	112.3	113.4	111.6	67.6	72.2
Am	106.2	109.5	115.1	118.2	119.4	67.2	72.2
Cm	105.6	108.6	110.8	114.1	111.9	68.4	73.1
Bk	105.0	107.7	109.3	114.6	114.1	68.9	73.8
Cf	109.2	104.8	106.2	117.5	114.4	65.3	73.0
Es	112.8	109.0	90.0	118.7	117.8	67.6	72.9
Fm	105.3	108.8	108.9	119.4	119.8	66.9	72.1
Md	119.9	119.9	117.4	115.5	113.6	64.5	69.7
No	-	119.4	119.7	119.9	119.9	65.6	71.6
Lr	109.3	112.7	115.4	118.5	119.3	70.7	75.6

2. Hirshfeld, VDD, NEC charges on An atoms

Table S4. Hirshfeld charges on An atom

Series	F	Cl	Br	I	At	PO ₄	AsO ₄
Ac	1.32	0.87	0.81	0.72	0.64	1.05	0.98
Th	0.78	0.56	0.48	0.39	0.33	0.77	-
Pa	0.80	0.63	0.58	0.50	0.44	0.82	-
U	0.81	0.64	0.59	0.52	0.46	0.84	0.77
Np	0.83	0.64	0.59	0.53	0.47	0.86	0.78
Pu	0.95	0.76	0.71	0.61	0.54	0.96	0.89
Am	0.98	0.78	0.69	0.60	0.53	0.96	0.90
Cm	0.92	0.70	0.63	0.56	0.49	0.90	0.84
Bk	1.01	0.79	0.73	0.64	0.58	0.74	0.91
Cf	1.01	0.75	0.68	0.63	0.54	0.90	0.89
Es	1.03	0.75	0.70	0.60	0.53	0.81	0.87
Fm	0.99	0.71	0.63	0.57	0.49	0.86	0.83
Md	1.00	0.71	0.62	0.51	0.45	0.13	0.85
No	-	0.70	0.62	0.52	0.47	0.88	0.82
Lr	1.00	0.75	0.68	0.60	0.54	0.98	0.91

Table S5. Voronoi Deformation Density (VDD) charges on An atom

Series	F	Cl	Br	I	At	PO ₄	AsO ₄
Ac	0.95	0.72	0.76	0.76	0.71	0.82	0.77
Th	0.24	0.44	0.47	0.45	0.41	0.58	-
Pa	0.41	0.56	0.58	0.55	0.51	0.64	-
U	0.44	0.58	0.61	0.59	0.54	0.64	0.60
Np	0.44	0.59	0.60	0.60	0.56	0.64	0.60
Pu	0.64	0.73	0.74	0.67	0.61	0.82	0.77
Am	0.67	0.74	0.72	0.66	0.61	0.83	0.79
Cm	0.54	0.65	0.67	0.63	0.58	0.75	0.70
Bk	0.74	0.79	0.78	0.71	0.65	0.59	0.83
Cf	0.74	0.76	0.74	0.69	0.62	0.78	0.81

Es	0.76	0.75	0.76	0.67	0.60	0.69	0.79
Fm	0.76	0.71	0.68	0.64	0.56	0.74	0.75
Md	0.73	0.69	0.65	0.57	0.52	0.90	0.77
No	-	0.69	0.66	0.60	0.55	0.78	0.74
Lr	0.71	0.76	0.75	0.70	0.64	0.89	0.83

Table S6. Natural Electronic Charges (NEC) on An atom

Series	F	Cl	Br	I	At	PO₄	AsO₄
Ac	2.41	1.73	1.59	1.41	1.31	2.02	2.00
Th	1.92	1.24	1.08	0.85	0.77	1.69	-
Pa	1.79	1.22	1.13	0.96	0.89	1.59	-
U	1.83	1.21	1.11	0.94	0.86	1.66	1.62
Np	1.85	1.28	1.18	1.03	0.96	1.70	1.66
Pu	1.93	1.38	1.30	1.08	0.99	1.72	1.69
Am	1.98	1.46	1.32	1.15	1.09	1.73	1.72
Cm	2.05	1.49	1.37	1.18	1.08	1.80	1.78
Bk	2.02	1.45	1.33	1.15	1.07	1.45	1.73
Cf	2.04	1.37	1.25	1.14	1.05	1.64	1.70
Es	2.05	1.41	1.27	1.13	1.05	1.54	1.67
Fm	1.99	1.37	1.22	1.09	1.04	1.58	1.62
Md	2.01	1.41	1.25	1.04	0.97	0.65	1.60
No	-	1.42	1.27	1.08	1.02	1.60	1.59
Lr	2.22	1.62	1.47	1.24	1.15	1.97	1.95

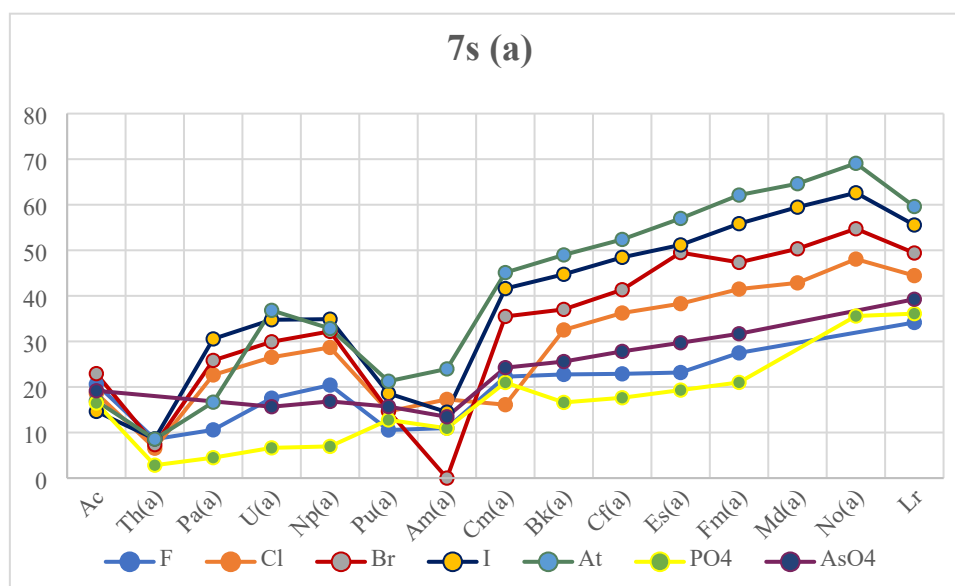
3. Wiberg Bond Indices

Table S7. Wiberg Bond Index (WBI) values for An-X & An-O (in phosphates and arsenates)

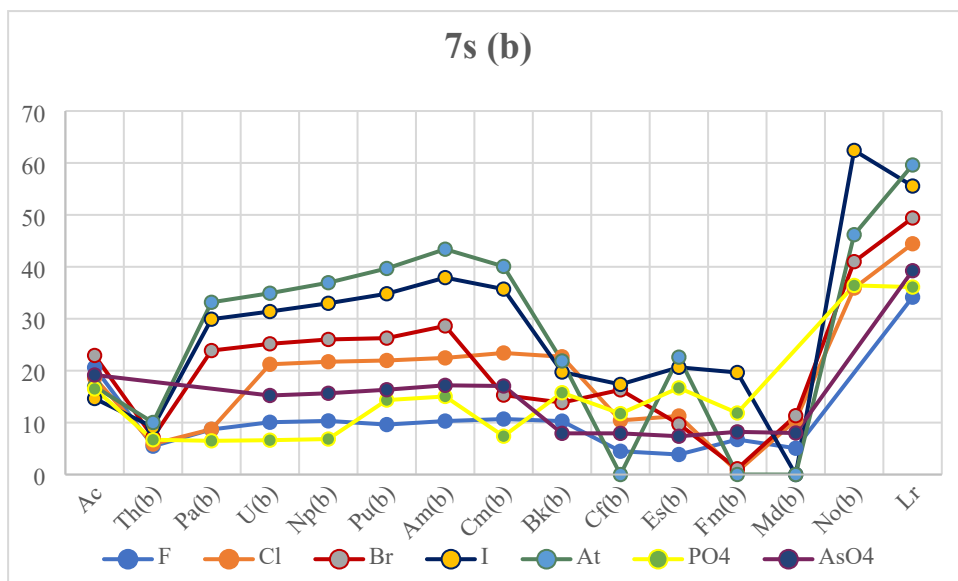
Series	F	Cl	Br	I	At	PO₄	AsO₄
Ac	0.37	0.76	0.83	0.91	0.96	0.55	0.57
Th	0.66	1.02	1.09	1.18	1.22	0.74	-

Pa	0.74	1.04	1.08	1.14	1.17	0.79	-
U	0.72	1.05	1.09	1.17	1.20	0.75	0.78
Np	0.71	1.01	1.06	1.11	1.14	0.74	0.77
Pu	0.65	0.93	0.99	1.06	1.09	0.71	0.74
Am	0.63	0.89	0.94	0.98	0.98	0.68	0.65
Cm	0.59	0.89	0.94	1.02	1.07	0.67	0.69
Bk	0.60	0.91	0.96	1.04	1.08	0.54	0.71
Cf	0.57	0.95	0.99	1.01	1.04	0.63	0.72
Es	0.58	0.93	0.92	0.98	1.02	0.53	0.71
Fm	0.60	0.93	0.99	1.00	0.95	0.64	0.71
Md	0.51	0.77	0.81	0.84	0.84	-	0.59
No	-	0.62	0.62	0.63	0.62	0.27	0.30
Lr	0.48	0.80	0.86	0.95	0.97	0.56	0.58

4. Natural Localized Molecular Orbitals (NLMO) Results

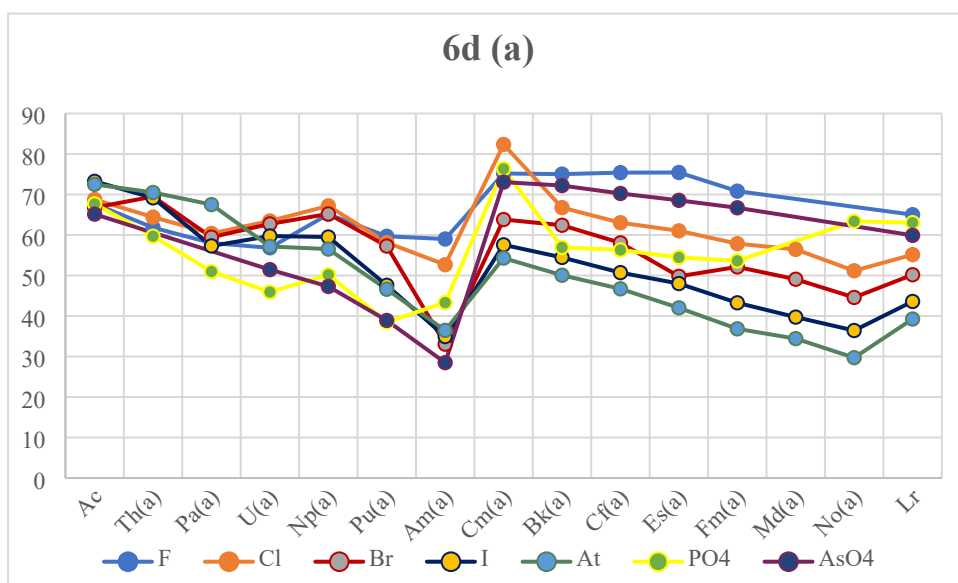


(a) denotes alpha spin contributions

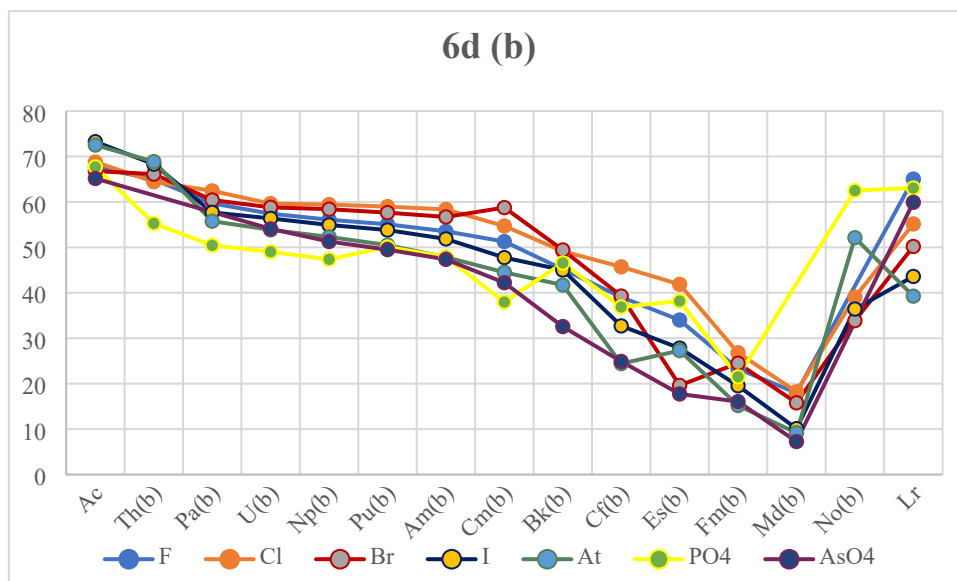


(b) denotes beta spin contributions

Figure S1. Percentage of average 7s orbital contributions from NLMO towards the bonding orbitals

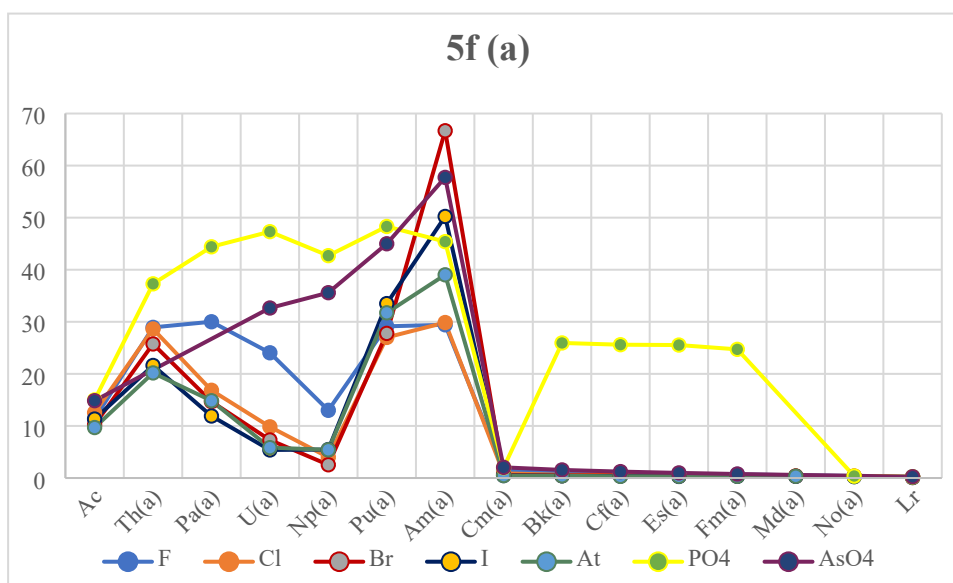


(a) denotes alpha spin contributions

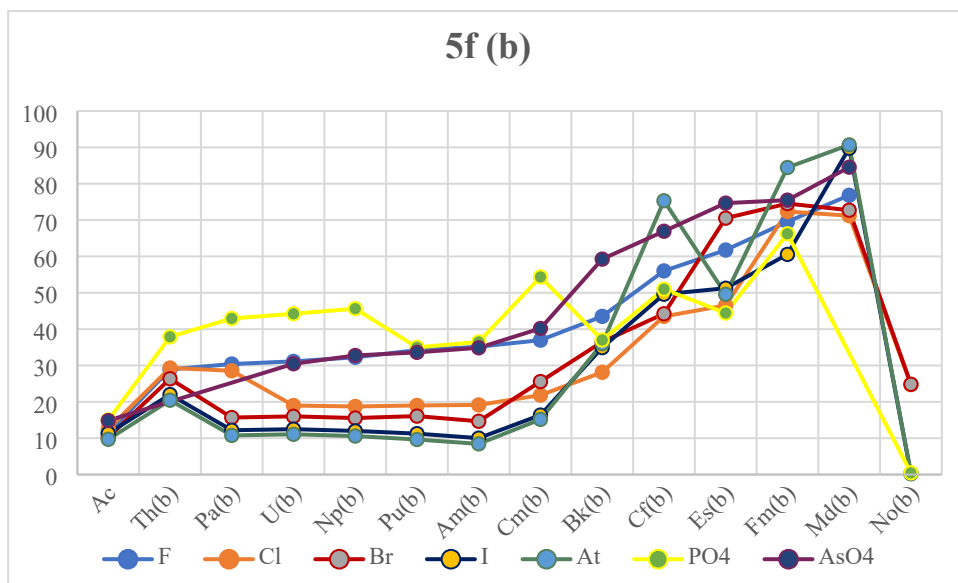


(b) denotes beta spin contributions

Figure S2. Percentage of average 6d orbital contributions from NLMO towards the bonding orbitals

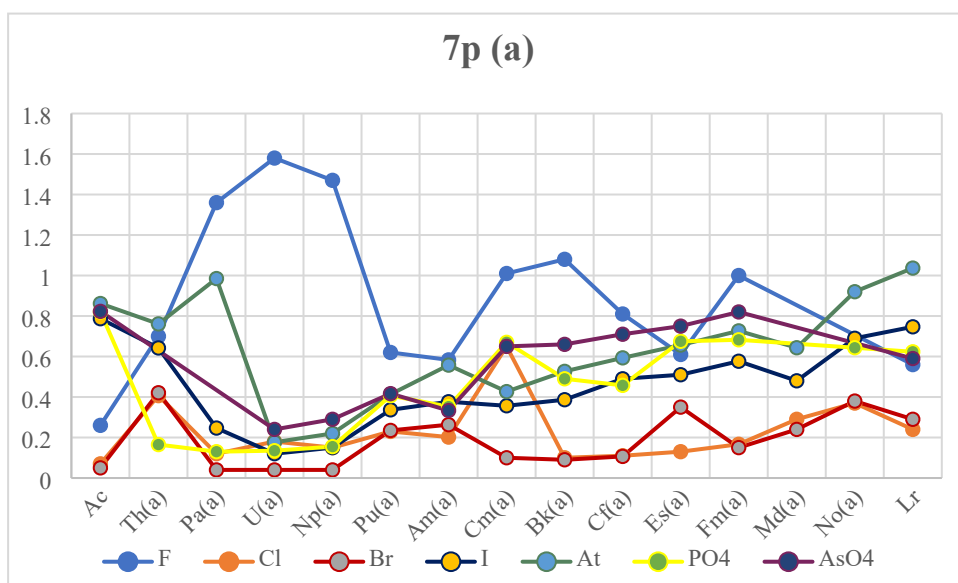


(a) denotes alpha spin contributions



(b) denotes beta spin contributions

Figure S3. Percentage of average 5f orbital contributions from NLMO towards the bonding orbitals



(a) denotes alpha spin contributions

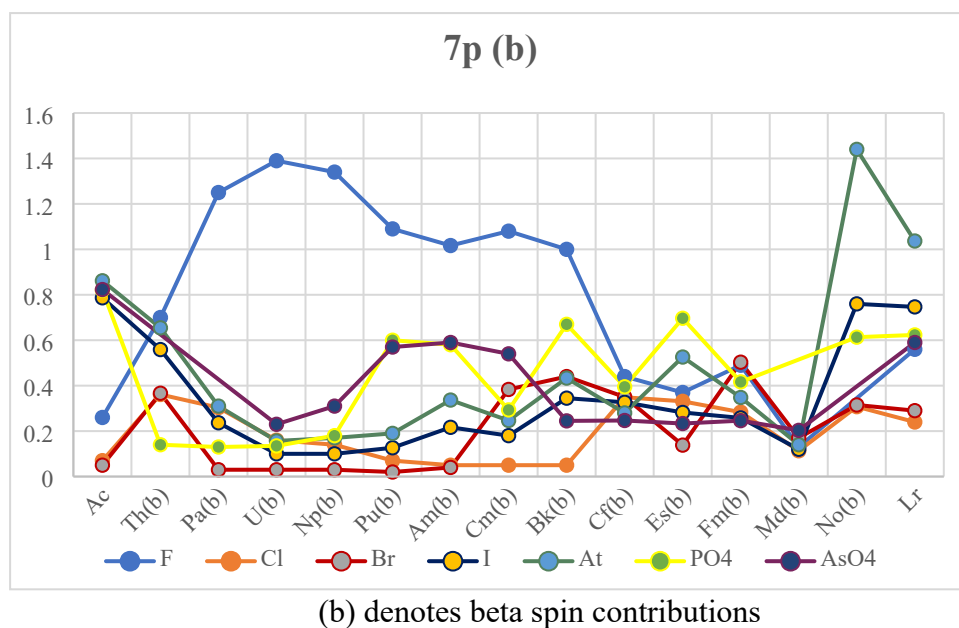


Figure S4. Percentage of average 7p orbital contributions from NLMO towards the bonding orbitals

5. Full reference for the Amsterdam Density Functional (ADF) software

ADF2017, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>.

E.J. Baerends, T. Ziegler, A.J. Atkins, J. Autschbach, O. Baseggio, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, C. Daul, D.P. Chong, D.V. Chulhai, L. Deng, R.M. Dickson, J.M. Dieterich, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A. Goetz, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, Z. Hu, C.R. Jacob, H. Jacobsen, L. Jensen, L. Joubert, J.W. Kaminski, G. van Kessel, C. König, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, C.A. Peeples, P.H.T. Philipsen, D. Post, C.C. Pye, H. Ramanantoanina, P. Ramos, W. Ravenek, J.I. Rodríguez, P. Ros, R. Rüger, P.R.T. Schipper, D. Schlüns, H. van Schoot, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Stener, M. Swart, D. Swerhone, V. Tognetti, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev

6. Electronic Configurations of An³⁺ for Scalar Relativistic DFT

Table S8. Electronic Configurations of An³⁺ for Scalar Relativistic DFT

An	G.S. Configuration	An ³⁺ Configuration
Ac	[Rn] 7s ² 6d ¹	[Rn]
Th	[Rn] 7s ² 6d ²	[Rn] 6d ¹
Pa	[Rn] 7s ² 5f ² 6d ¹	[Rn] 5f ²
U	[Rn] 7s ² 5f ³ 6d ¹	[Rn] 5f ³
Np	[Rn] 7s ² 5f ⁴ 6d ¹	[Rn] 5f ⁴
Pu	[Rn] 7s ² 5f ⁶	[Rn] 5f ⁵
Am	[Rn] 7s ² 5f ⁷	[Rn] 5f ⁶
Cm	[Rn] 7s ² 5f ⁷ 6d ¹	[Rn] 5f ⁷
Bk	[Rn] 7s ² 5f ⁹	[Rn] 5f ⁸
Cf	[Rn] 7s ² 5f ¹⁰	[Rn] 5f ⁹
Es	[Rn] 7s ² 5f ¹¹	[Rn] 5f ¹⁰
Fm	[Rn] 7s ² 5f ¹²	[Rn] 5f ¹¹
Md	[Rn] 7s ² 5f ¹³	[Rn] 5f ¹²
No	[Rn] 7s ² 5f ¹⁴	[Rn] 5f ¹³
Lr	[Rn] 7s ² 5f ¹⁴ 7p ¹	[Rn] 5f ¹⁴

7. Cartesian Coordinates (Angstroms) and Frequencies (cm⁻¹) of Optimized Geometries

Cartesian Coordinates (Angstroms) and Frequencies (cm⁻¹) of Optimized Geometries (SR)

[AcF₃]

	X	Y	Z
Ac	0.000000000	0.000000000	-0.355987000
F	-1.038698000	-1.799078000	0.345756000
F	2.077396000	0.000000000	0.345756000
F	-1.038698000	1.799078000	0.345756000

Frequencies (cm⁻¹)

1	76.611
2	106.214
3	106.214
4	467.913
5	467.913
6	505.627

[ThF₃]

	X	Y	Z
Th	0.000000000000	0.000000000000	-0.052465000000
F	-1.051173000000	-1.820686000000	-0.013138000000
F	-1.051173000000	1.820686000000	-0.013138000000
F	2.102347000000	0.000000000000	-0.013138000000

Frequencies (cm⁻¹)

1	44.458
2	95.092
3	95.092
4	534.079
5	534.079
6	562.882

[PaF₃]

	X	Y	Z
Pa	0.000000000000	0.000000000000	-0.226571000000
F	-0.953924000000	-1.652244000000	0.556067000000
F	-0.953924000000	1.652244000000	0.556067000000
F	1.907847000000	0.000000000000	0.556067000000

Frequencies (cm⁻¹)

1	89.157
2	93.862
3	93.862
4	516.732
5	516.732
6	569.497

[UF₃]

	X	Y	Z
U	0.000000000000	0.000000000000	0.284534000000

F	-1.859942000000	0.000000000000	-0.606154000000
F	0.929971000000	-1.610757000000	-0.606154000000
F	0.929971000000	1.610757000000	-0.606154000000

Frequencies (cm⁻¹)

1	111.136
2	170.024
3	170.024
4	559.368
5	570.858
6	570.858

[NpF₃]

	X	Y	Z
Np	-0.751151000000	-0.989676000000	0.000000000000
F	-2.576034000000	-1.945543000000	0.000000000000
F	0.200367000000	-1.866017000000	-1.603312000000
F	0.200367000000	-1.866017000000	1.603312000000

Frequencies (cm⁻¹)

1	113.362
2	122.845
3	123.029
4	530.214
5	530.285
6	551.991

[PuF₃]

	X	Y	Z
Pu	0.000000000000	0.000000000000	-0.143971000000
F	-0.952864000000	-1.650408000000	-0.943121000000
F	1.905727000000	0.000000000000	-0.943121000000
F	-0.952864000000	1.650408000000	-0.943121000000

Frequencies (cm⁻¹)

1	115.384
2	115.384
3	155.067
4	526.627
5	526.627
6	548.389

[AmF₃]

	X	Y	Z
Am	-0.495131000000	-0.030499000000	0.048813000000
F	0.672973000000	-1.693709000000	-0.350185000000
F	-2.085295000000	-0.699880000000	1.196454000000
F	0.640669000000	1.192557000000	1.275308000000

Frequencies (cm⁻¹)

1	110.133
2	140.031
3	140.273
4	510.477
5	511.187
6	553.025

[CmF₃]

	X	Y	Z
Cm	0.000000000000	0.000000000000	-0.713389000000
F	-1.898934000000	0.000000000000	-1.521257000000
F	0.949467000000	-1.644525000000	-1.521257000000
F	0.949467000000	1.644525000000	-1.521257000000

Frequencies (cm⁻¹)

1	104.708
2	137.186
3	137.186
4	523.225
5	523.225
6	555.285

[BkF₃]

	X	Y	Z
Bk	0.000000000000	0.000000000000	-0.168667000000
F	-0.938995000000	1.626387000000	0.650108000000
F	-0.938995000000	-1.626387000000	0.650108000000
F	1.877990000000	0.000000000000	0.650108000000

Frequencies (cm⁻¹)

1	111.117
2	134.196
3	134.196
4	523.356
5	523.356
6	560.270

[CfF₃]

	X	Y	Z
Cf	0.000000000000	0.000000000000	-0.111235000000
F	-0.965162000000	1.671709000000	0.579606000000
F	-0.965162000000	-1.671709000000	0.579606000000
F	1.930323000000	0.000000000000	0.579606000000

Frequencies (cm⁻¹)

1	131.926
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2	141.701
3	141.701
4	524.282
5	524.282
6	551.460

[EsF₃]

	X	Y	Z
Es	0.000000000000	0.000000000000	-0.478280000000
F	-0.985867000000	1.707572000000	-1.037958000000
F	1.971734000000	0.000000000000	-1.037958000000
F	-0.985867000000	-1.707572000000	-1.037958000000

Frequencies (cm⁻¹)

1	80.570
2	103.526
3	103.526
4	520.908
5	520.908
6	542.017

[FmF₃]

	X	Y	Z
Fm	0.000000000000	0.000000000000	-0.191104000000
F	-0.938481000000	1.625497000000	0.618706000000
F	-0.938481000000	-1.625497000000	0.618706000000
F	1.876962000000	0.000000000000	0.618706000000

Frequencies (cm⁻¹)

1	81.761
2	149.631
3	149.631
4	515.335
5	515.335
6	533.441

[MdF₃]

	X	Y	Z
Md	0.000000000000	0.000000000000	-0.379614000000
F	-1.034628000000	1.792028000000	-0.403753000000
F	2.069256000000	0.000000000000	-0.403753000000
F	-1.034628000000	-1.792028000000	-0.403753000000

Frequencies (cm⁻¹)

1	79.230
2	79.230
3	108.368
4	492.296

5 492.296
6 497.592

[LrF₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	-0.050556000000
F	-0.952262000000	1.649367000000	0.628754000000
F	-0.952262000000	-1.649367000000	0.628754000000
F	1.904525000000	0.000000000000	0.628754000000

Frequencies (cm⁻¹)

1 100.634
2 149.423
3 149.423
4 551.167
5 551.167
6 572.867

[AcCl₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	-0.358341000000
Cl	-1.284504000000	-2.224826000000	0.362779000000
Cl	2.569008000000	0.000000000000	0.362779000000
Cl	-1.284504000000	2.224826000000	0.362779000000

Frequencies (cm⁻¹)

1 37.579
2 61.876
3 61.876
4 292.726
5 292.726
6 298.409

[ThCl₃]

	X	Y	Z
Th	0.144538000000	-0.580706000000	-0.509828000000
Cl	0.210361000000	-3.127475000000	-0.283614000000
Cl	-2.088475000000	0.607317000000	-0.887198000000
Cl	2.315337000000	0.766531000000	-0.403553000000

Frequencies (cm⁻¹)

1 40.365
2 57.759
3 58.131
4 325.789
5 326.085
6 327.915

[PaCl₃]

	X	Y	Z
Pa	0.000000000000	0.000000000000	-0.203336000000
Cl	-1.207273000000	-2.091058000000	0.536732000000
Cl	-1.207273000000	2.091058000000	0.536732000000
Cl	2.414546000000	0.000000000000	0.536732000000

Frequencies (cm⁻¹)

1	46.188
2	59.02
3	59.02
4	319.831
5	319.938
6	319.938

[UCl₃]

	X	Y	Z
U	0.000000000000	0.000000000000	0.275636000000
Cl	-2.317419000000	0.000000000000	-0.687906000000
Cl	1.158709000000	-2.006944000000	-0.687906000000
Cl	1.158709000000	2.006944000000	-0.687906000000

Frequencies (cm⁻¹)

1	70.34
2	80.683
3	80.683
4	321.139
5	321.139
6	322.022

[NpCl₃]

	X	Y	Z
Np	-0.750893000000	-1.004935000000	0.000000000000
Cl	-3.047121000000	-2.014822000000	0.000000000000
Cl	0.438810000000	-1.915306000000	-2.009732000000
Cl	0.438810000000	-1.915306000000	2.009732000000

Frequencies (cm⁻¹)

1	56.542
2	70.643
3	70.828
4	315.481
5	316.305
6	319.268

[PuCl₃]

	X	Y	Z
Pu	0.000000000000	0.000000000000	-0.158573000000

Cl	-1.185011000000	-2.052500000000	-0.969635000000
Cl	2.370022000000	0.000000000000	-0.969635000000
Cl	-1.185011000000	2.052500000000	-0.969635000000

Frequencies (cm⁻¹)

1	66.319
2	66.319
3	77.344
4	314.558
5	314.625
6	314.625

[AmCl₃]

	X	Y	Z
Am	-0.281975000000	0.064892000000	0.000000000000
Cl	1.741141000000	-1.416281000000	0.000000000000
Cl	-1.433273000000	-0.083689000000	-2.236409000000
Cl	-1.433273000000	-0.083689000000	2.236409000000

Frequencies (cm⁻¹)

1	28.92
2	32.729
3	44.658
4	297.251
5	305.532
6	306.130

[CmCl₃]

	X	Y	Z
Cm	0.000000000000	0.000000000000	-0.710170000000
Cl	-2.331898000000	0.000000000000	-1.571971000000
Cl	1.165949000000	-2.019483000000	-1.571971000000
Cl	1.165949000000	2.019483000000	-1.571971000000

Frequencies (cm⁻¹)

1	55.15
2	76.699
3	76.699
4	316.238
5	316.238
6	321.492

[BkCl₃]

	X	Y	Z
Bk	0.000000000000	0.000000000000	-0.173098000000
Cl	-1.152797000000	1.996702000000	0.716578000000
Cl	-1.152797000000	-1.996702000000	0.716578000000
Cl	2.305593000000	0.000000000000	0.716578000000

Frequencies (cm⁻¹)

1	57.778
2	73.533
3	73.533
4	314.59
5	314.59
6	321.026

[CfCl₃]

	X	Y	Z
Cf	0.000000000000	0.000000000000	-0.169625000000
Cl	-1.125115000000	1.948756000000	0.819924000000
Cl	-1.125115000000	-1.948756000000	0.819924000000
Cl	2.250230000000	0.000000000000	0.819924000000

Frequencies (cm⁻¹)

1	62.017
2	70.267
3	70.267
4	313.523
5	313.523
6	314.141

[EsCl₃]

	X	Y	Z
Es	0.000000000000	0.000000000000	-0.424786000000
Cl	-1.160752000000	2.010481000000	-1.263756000000
Cl	2.321504000000	0.000000000000	-1.263756000000
Cl	-1.160752000000	-2.010481000000	-1.263756000000

Frequencies (cm⁻¹)

1	43.544
2	142.632
3	142.632
4	298.566
5	327.064
6	327.064

[FmCl₃]

	X	Y	Z
Fm	0.000000000000	0.000000000000	-0.110653000000
Cl	-1.168276000000	2.023514000000	0.745232000000
Cl	-1.168276000000	-2.023514000000	0.745232000000
Cl	2.336552000000	0.000000000000	0.745232000000

Frequencies (cm⁻¹)

1	36.497
---	--------

2	50.405
3	50.405
4	275.381
5	275.381
6	282.221

[MdCl₃]

	X	Y	Z
Md	0.000000000000	0.000000000000	0.132527000000
Cl	-1.255019000000	2.173756000000	0.144767000000
Cl	-1.255019000000	-2.173756000000	0.144767000000
Cl	2.510037000000	0.000000000000	0.144767000000

Frequencies (cm⁻¹)

1	53.536
2	53.536
3	61.316
4	260.475
5	273.941
6	273.941

[NoCl₃]

	X	Y	Z
No	0.000000000000	0.000000000000	0.081667000000
Cl	-1.270932000000	2.201320000000	0.265608000000
Cl	-1.270932000000	-2.201320000000	0.265608000000
Cl	2.541865000000	0.000000000000	0.265608000000

Frequencies (cm⁻¹)

1	13.963
2	23.659
3	23.659
4	239.939
5	245.053
6	245.053

[LrCl₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	-0.058543000000
Cl	-1.170634000000	2.027597000000	0.608867000000
Cl	-1.170634000000	-2.027597000000	0.608867000000
Cl	2.341267000000	0.000000000000	0.608867000000

Frequencies (cm⁻¹)

1	48.609
2	82.501
3	82.501
4	327.971

5 329.711
6 329.711

[AcBr₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	0.389169000000
Br	-1.366614000000	-2.367046000000	1.105913000000
Br	2.733229000000	0.000000000000	1.105913000000
Br	-1.366614000000	2.367046000000	1.105913000000

Frequencies (cm⁻¹)

1 25.222
2 39.729
3 39.729
4 188.809
5 204.123
6 204.123

[ThBr₃]

	X	Y	Z
Th	0.000000000000	0.000000000000	0.763082000000
Br	-1.356290000000	-2.349163000000	0.765921000000
Br	2.712579000000	0.000000000000	0.765921000000
Br	-1.356290000000	2.349163000000	0.765921000000

Frequencies (cm⁻¹)

1 31.381
2 37.813
3 37.813
4 202.522
5 226.908
6 226.908

[PaBr₃]

	X	Y	Z
Pa	0.000000000000	0.000000000000	-0.131531000000
Br	-1.300687000000	-2.252856000000	0.538336000000
Br	-1.300687000000	2.252856000000	0.538336000000
Br	2.601374000000	0.000000000000	0.538336000000

Frequencies (cm⁻¹)

1 29.025
2 37.924
3 37.924
4 200.166
5 222.758
6 222.758

[UBr₃]

	X	Y	Z
U	0.000000000000	0.000000000000	0.222350000000
Br	-2.509942000000	0.000000000000	-0.707370000000
Br	1.254971000000	-2.173674000000	-0.707370000000
Br	1.254971000000	2.173674000000	-0.707370000000

Frequencies (cm⁻¹)

1	39.078
2	44.85
3	44.85
4	203.195
5	216.594
6	216.594

[NpBr₃]

	X	Y	Z
Np	-0.749366000000	-1.043943000000	0.000000000000
Br	-3.219787000000	-2.049281000000	0.000000000000
Br	0.526808000000	-1.942638000000	-2.162528000000
Br	0.526808000000	-1.942638000000	2.162528000000

Frequencies (cm⁻¹)

1	36.464
2	44.301
3	44.315
4	203.233
5	215.962
6	215.986

[PuBr₃]

	X	Y	Z
Pu	0.000000000000	0.000000000000	-0.221693000000
Br	-1.278788000000	-2.214926000000	-0.977448000000
Br	2.557576000000	0.000000000000	-0.977448000000
Br	-1.278788000000	2.214926000000	-0.977448000000

Frequencies (cm⁻¹)

1	41.043
2	41.043
3	48.574
4	195.862
5	214.09
6	214.09

[AmBr₃]

X	Y	Z
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Am	0.000000000000	0.000000000000	-1.298003000000
Br	-1.305814000000	2.261736000000	-1.895741000000
Br	2.611627000000	0.000000000000	-1.895741000000
Br	-1.305814000000	-2.261736000000	-1.895741000000

Frequencies (cm⁻¹)

1	6.125
2	6.125
3	26.296
4	181.816
5	205.219
6	205.219

[CmBr₃]

	X	Y	Z
Cm	0.000000000000	0.000000000000	-0.798854000000
Br	-2.513862000000	0.000000000000	-1.616013000000
Br	1.256931000000	-2.177068000000	-1.616013000000
Br	1.256931000000	2.177068000000	-1.616013000000

Frequencies (cm⁻¹)

1	34.008
2	47.709
3	47.709
4	201.756
5	215.839
6	215.839

[BkBr₃]

	X	Y	Z
Bk	0.000000000000	0.000000000000	-0.104161000000
Br	-1.237947000000	2.144187000000	0.777395000000
Br	-1.237947000000	-2.144187000000	0.777395000000
Br	2.475894000000	0.000000000000	0.777395000000

Frequencies (cm⁻¹)

1	36.48
2	45.049
3	45.049
4	201.89
5	214.057
6	214.057

[CfBr₃]

	X	Y	Z
Cf	0.000000000000	0.000000000000	-0.072177000000
Br	-1.213746000000	2.102269000000	0.934715000000
Br	-1.213746000000	-2.102269000000	0.934715000000

Br	2.427491000000	0.000000000000	0.934715000000
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Frequencies (cm⁻¹)

1	40.51
2	61.716
3	61.716
4	196.747
5	209.56
6	209.56

[EsBr₃]

	X	Y	Z
Es	0.000000000000	0.000000000000	-0.801378000000
Br	-1.251134000000	2.167027000000	-1.614341000000
Br	2.502267000000	0.000000000000	-1.614341000000
Br	-1.251134000000	-2.167027000000	-1.614341000000

Frequencies (cm⁻¹)

1	37.515
2	39.732
3	39.732
4	184.06
5	202.001
6	202.001

[FmBr₃]

	X	Y	Z
Fm	0.000000000000	0.000000000000	-0.026775000000
Br	-1.245974000000	2.158091000000	0.878310000000
Br	-1.245974000000	-2.158091000000	0.878310000000
Br	2.491948000000	0.000000000000	0.878310000000

Frequencies (cm⁻¹)

1	26.303
2	27.514
3	27.514
4	175.095
5	184.349
6	184.349

[MdBr₃]

	X	Y	Z
Md	0.000000000000	0.000000000000	-0.190740000000
Br	-1.321275000000	2.288515000000	-0.619321000000
Br	-1.321275000000	-2.288515000000	-0.619321000000
Br	2.642550000000	0.000000000000	-0.619321000000

Frequencies (cm⁻¹)

1	30.558
2	30.558
3	43.649
4	157.994
5	180.569
6	180.569

[NoBr₃]

	X	Y	Z
No	0.000000000000	0.000000000000	-0.611507000000
Br	-1.357408000000	2.351100000000	-0.747721000000
Br	-1.357408000000	-2.351100000000	-0.747721000000
Br	2.714816000000	0.000000000000	-0.747721000000

Frequencies (cm⁻¹)

1	12.872
2	18.366
3	18.366
4	143.968
5	162.749
6	162.749

[LrBr₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	0.086158000000
Br	-1.263060000000	2.187684000000	0.643356000000
Br	-1.263060000000	-2.187684000000	0.643356000000
Br	2.526120000000	0.000000000000	0.643356000000

Frequencies (cm⁻¹)

1	25.751
2	51.325
3	51.325
4	202.442
5	224.646
6	224.646

[AcI₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	0.551158000000
I	-1.499823000000	-2.597770000000	1.137261000000
I	2.999647000000	0.000000000000	1.137261000000
I	-1.499823000000	2.597770000000	1.137261000000

Frequencies (cm⁻¹)

1	13.985
2	28.274
3	28.274

4	134.778
5	164.938
6	164.938

[ThI₃]

	X	Y	Z
Th	0.000000000000	0.000000000000	0.765199000000
I	-1.468331000000	-2.543223000000	0.765057000000
I	2.936661000000	0.000000000000	0.765057000000
I	-1.468331000000	2.543223000000	0.765057000000

Frequencies (cm⁻¹)

1	26.844
2	27.067
3	27.067
4	144.131
5	181.273
6	181.273

[PaI₃]

	X	Y	Z
Pa	0.000000000000	0.000000000000	-0.051398000000
I	-1.424139000000	-2.466680000000	0.557975000000
I	-1.424139000000	2.466680000000	0.557975000000
I	2.848277000000	0.000000000000	0.557975000000

Frequencies (cm⁻¹)

1	18.66
2	27.669
3	27.669
4	144.204
5	178.149
6	178.149

[UI₃]

	X	Y	Z
U	0.000000000000	0.000000000000	0.187115000000
I	-2.743833000000	0.000000000000	-0.759463000000
I	1.371917000000	-2.376229000000	-0.759463000000
I	1.371917000000	2.376229000000	-0.759463000000

Frequencies (cm⁻¹)

1	28.317
2	32.282
3	32.282
4	148.746
5	171.822
6	171.822

[NpI₃]

	X	Y	Z
Np	0.000000000000	0.000000000000	0.970180000000
I	-2.694060000000	0.000000000000	2.033087000000
I	1.347030000000	-2.333125000000	2.033087000000
I	1.347030000000	2.333125000000	2.033087000000

Frequencies (cm⁻¹)

1	30.46
2	33.319
3	33.319
4	151.772
5	169.333
6	169.333

[PuI₃]

	X	Y	Z
Pu	0.000000000000	0.000000000000	-0.264600000000
I	-1.396293000000	-2.418450000000	-1.021673000000
I	2.792586000000	0.000000000000	-1.021673000000
I	-1.396293000000	2.418450000000	-1.021673000000

Frequencies (cm⁻¹)

1	28.375
2	28.375
3	35.235
4	139.498
5	167.863
6	167.863

[AmI₃]

	X	Y	Z
Am	0.000000000000	0.000000000000	-1.474788000000
I	-1.447012000000	2.506297000000	-1.867872000000
I	2.894023000000	0.000000000000	-1.867872000000
I	-1.447012000000	-2.506297000000	-1.867872000000

Frequencies (cm⁻¹)

1	13.866
2	13.866
3	13.92
4	122.49
5	156.939
6	156.939

[CmI₃]

	X	Y	Z
Cm	0.000000000000	0.000000000000	-0.946577000000
I	-2.782496000000	0.000000000000	-1.652070000000
I	1.391248000000	-2.409712000000	-1.652070000000
I	1.391248000000	2.409712000000	-1.652070000000

Frequencies (cm⁻¹)

1	21.049
2	32.712
3	32.712
4	142.125
5	170.368
6	170.368

[BkI₃]

	X	Y	Z
Bk	0.000000000000	0.000000000000	0.105290000000
I	-1.390092000000	2.407709000000	0.776297000000
I	-1.390092000000	-2.407709000000	0.776297000000
I	2.780183000000	0.000000000000	0.776297000000

Frequencies (cm⁻¹)

1	19.066
2	28.283
3	28.283
4	137.825
5	168.306
6	168.306

[CfI₃]

	X	Y	Z
Cf	0.000000000000	0.000000000000	0.391095000000
I	-1.421313000000	2.461786000000	0.844596000000
I	-1.421313000000	-2.461786000000	0.844596000000
I	2.842626000000	0.000000000000	0.844596000000

Frequencies (cm⁻¹)

1	12.873
2	17.63
3	17.63
4	126.696
5	159.173
6	159.173

[EsI₃]

	X	Y	Z
Es	0.000000000000	0.000000000000	-1.334805000000

I	-1.432425000000	2.481033000000	-1.653011000000
I	2.864850000000	0.000000000000	-1.653011000000
I	-1.432425000000	-2.481033000000	-1.653011000000

Frequencies (cm⁻¹)

1	8.726
2	8.726
3	12.82
4	119.289
5	153.5
6	153.5

[FmI₃]

	X	Y	Z
Fm	0.000000000000	0.000000000000	0.521417000000
I	-1.448960000000	2.509673000000	0.739976000000
I	-1.448960000000	-2.509673000000	0.739976000000
I	2.897920000000	0.000000000000	0.739976000000

Frequencies (cm⁻¹)

1	21.755
2	21.755
3	31.081
4	112.999
5	144.518
6	144.518

[MdI₃]

	X	Y	Z
Md	0.000000000000	0.000000000000	-0.138041000000
I	-1.426677000000	2.471076000000	-0.759562000000
I	-1.426677000000	-2.471076000000	-0.759562000000
I	2.853353000000	0.000000000000	-0.759562000000

Frequencies (cm⁻¹)

1	17.609
2	17.609
3	32.418
4	111.19
5	134.546
6	134.546

[NoI₃]

	X	Y	Z
No	0.000000000000	0.000000000000	-0.679195000000
I	-1.476692000000	2.557706000000	-0.732329000000
I	-1.476692000000	-2.557706000000	-0.732329000000
I	2.953384000000	0.000000000000	-0.732329000000

Frequencies (cm⁻¹)

1	9.483
2	9.483
3	9.636
4	101.333
5	124.968
6	124.968

[LrI₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	0.310320000000
I	-1.395233000000	2.416615000000	0.650344000000
I	-1.395233000000	-2.416615000000	0.650344000000
I	2.790466000000	0.000000000000	0.650344000000

Frequencies (cm⁻¹)

1	10.191
2	35.234
3	35.234
4	140.478
5	176.252
6	176.252

[AcAt₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	0.463323000000
At	-1.524716000000	-2.640885000000	1.234806000000
At	3.049432000000	0.000000000000	1.234806000000
At	-1.524716000000	2.640885000000	1.234806000000

Frequencies (cm⁻¹)

1	15.404
2	21.555
3	21.555
4	105.325
5	137.805
6	137.805

[ThAt₃]

	X	Y	Z
Th	0.000000000000	0.000000000000	0.000000000000
At	-3.025059000000	0.000000000000	0.000000000000
At	1.512530000000	-2.619778000000	0.000000000000
At	1.512530000000	2.619778000000	0.000000000000

Frequencies (cm⁻¹)

1	19.867
---	--------

2	19.867
3	23.218
4	106.503
5	152.734
6	152.734

[PaAt₃]

	X	Y	Z
Pa	0.000000000000	0.000000000000	-0.051398000000
I	-1.424139000000	-2.466680000000	0.557975000000
I	-1.424139000000	2.466680000000	0.557975000000
I	2.848277000000	0.000000000000	0.557975000000

Frequencies (cm⁻¹)

1	18.66
2	27.669
3	27.669
4	144.204
5	178.149
6	178.149

[UAt₃]

	X	Y	Z
U	0.000000000000	0.000000000000	0.229073000000
At	-2.810932000000	0.000000000000	-0.794062000000
At	1.405466000000	-2.434339000000	-0.794062000000
At	1.405466000000	2.434339000000	-0.794062000000

Frequencies (cm⁻¹)

1	24.197
2	25.024
3	25.024
4	117.071
5	142.407
6	142.407

[NpAt₃]

	X	Y	Z
Np	0.000000000000	0.000000000000	0.964861000000
At	-2.774881000000	0.000000000000	2.077140000000
At	1.387440000000	-2.403117000000	2.077140000000
At	1.387440000000	2.403117000000	2.077140000000

Frequencies (cm⁻¹)

1	25.5
2	25.549
3	25.549
4	119.225

5 139.43
6 139.43

[PuAt₃]

	X	Y	Z
Pu	0.000000000000	0.000000000000	-0.192051000000
At	-1.427709000000	-2.472865000000	-1.075050000000
At	2.855418000000	0.000000000000	-1.075050000000
At	-1.427709000000	2.472865000000	-1.075050000000

Frequencies (cm⁻¹)

1 22.021
2 22.021
3 30.842
4 107.797
5 137.07
6 137.07

[AmAt₃]

	X	Y	Z
Am	0.000000000000	0.000000000000	-1.617172000000
At	-1.507773000000	2.611539000000	-1.841136000000
At	3.015546000000	0.000000000000	-1.841136000000
At	-1.507773000000	-2.611539000000	-1.841136000000

Frequencies (cm⁻¹)

1 7.595
2 10.185
3 10.185
4 87.603
5 128.988
6 128.988

[CmAt₃]

	X	Y	Z
Cm	0.000000000000	0.000000000000	-0.883624000000
At	-2.831127000000	0.000000000000	-1.742976000000
At	1.415564000000	-2.451828000000	-1.742976000000
At	1.415564000000	2.451828000000	-1.742976000000

Frequencies (cm⁻¹)

1 20.568
2 25.292
3 25.292
4 111.336
5 140.622
6 140.622

[BkAt₃]

	X	Y	Z
Bk	0.000000000000	0.000000000000	0.120316000000
At	-1.432331000000	2.480870000000	0.847656000000
At	-1.432331000000	-2.480870000000	0.847656000000
At	2.864662000000	0.000000000000	0.847656000000

Frequencies (cm⁻¹)

1	17.065
2	21.188
3	21.188
4	104.02
5	138.242
6	138.242

[CfAt₃]

	X	Y	Z
Cf	0.000000000000	0.000000000000	0.313364000000
At	-1.444258000000	2.501529000000	1.023241000000
At	-1.444258000000	-2.501529000000	1.023241000000
At	2.888516000000	0.000000000000	1.023241000000

Frequencies (cm⁻¹)

1	12.065
2	12.065
3	15.238
4	97.035
5	129.099
6	129.099

[EsAt₃]

	X	Y	Z
Es	0.000000000000	0.000000000000	-1.445951000000
At	-1.475437000000	2.555532000000	-1.889047000000
At	2.950874000000	0.000000000000	-1.889047000000
At	-1.475437000000	-2.555532000000	-1.889047000000

Frequencies (cm⁻¹)

1	8.211
2	8.211
3	12.587
4	87.303
5	125.132
6	125.132

[FmAt₃]

X	Y	Z
---	---	---

Fm	0.000000000000	0.000000000000	0.612266000000
At	-1.503918000000	2.604863000000	0.740056000000
At	-1.503918000000	-2.604863000000	0.740056000000
At	3.007837000000	0.000000000000	0.740056000000

Frequencies (cm⁻¹)

1	15.576
2	15.576
3	26.936
4	81.427
5	118.499
6	118.499

[MdAt₃]

	X	Y	Z
Md	0.000000000000	0.000000000000	-0.102103000000
At	-1.461159000000	2.530802000000	-0.876383000000
At	-1.461159000000	-2.530802000000	-0.876383000000
At	2.922318000000	0.000000000000	-0.876383000000

Frequencies (cm⁻¹)

1	11.409
2	11.409
3	26.299
4	84.723
5	109.092
6	109.092

[NoAt₃]

	X	Y	Z
No	0.000000000000	0.000000000000	-0.708428000000
At	-1.529011000000	2.648324000000	-0.728336000000
At	-1.529011000000	-2.648324000000	-0.728336000000
At	3.058021000000	0.000000000000	-0.728336000000

Frequencies (cm⁻¹)

1	5.587
2	5.587
3	9.144
4	73.882
5	103.075
6	103.075

[LrAt₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	0.429278000000
At	-1.448917000000	2.509598000000	0.672481000000
At	-1.448917000000	-2.509598000000	0.672481000000

At 2.897834000000 0.000000000000 0.672481000000
 Frequencies (cm⁻¹)

1 6.052
 2 26.258
 3 26.258
 4 102.143
 5 145.844
 6 145.844

[AcPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.510501000000
O	-1.412059000000	0.000000000000	-1.357943000000
O	0.706030000000	1.222879000000	-1.357943000000
O	0.706030000000	-1.222879000000	-1.357943000000
O	0.000000000000	0.000000000000	0.964822000000
Ac	0.000000000000	0.000000000000	-3.142995000000

Frequencies (cm⁻¹)

1 180.006
 2 180.006
 3 370.133
 4 379.352
 5 379.352
 6 498.755
 7 498.755
 8 620.306
 9 750.917
 10 750.917
 11 774.071
 12 1301.22

[ThPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.482412000000
O	-1.387506000000	0.000000000000	-1.380846000000
O	0.693753000000	1.201615000000	-1.380846000000
O	0.693753000000	-1.201615000000	-1.380846000000
O	0.000000000000	0.000000000000	0.985983000000
Th	0.000000000000	0.000000000000	-3.077598000000

Frequencies (cm⁻¹)

1 164.67
 2 164.67
 3 364.777
 4 364.777
 5 388.548
 6 497.459

7	497.459
8	632.749
9	753.551
10	753.551
11	776.749
12	1328.335

[PaPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.468148000000
O	-1.391044000000	0.000000000000	-1.360863000000
O	0.695522000000	1.204680000000	-1.360863000000
O	0.695522000000	-1.204680000000	-1.360863000000
O	0.000000000000	0.000000000000	0.999442000000
Pa	0.000000000000	0.000000000000	-3.024308000000

Frequencies (cm⁻¹)

1	157.547
2	157.547
3	359.292
4	359.292
5	375.266
6	489.504
7	489.504
8	639.376
9	756.901
10	756.901
11	772.177
12	1331.703

[UPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.441675000000
O	-1.393765000000	0.000000000000	-1.325460000000
O	0.696883000000	1.207036000000	-1.325460000000
O	0.696883000000	-1.207036000000	-1.325460000000
O	0.000000000000	0.000000000000	1.028794000000
U	0.000000000000	0.000000000000	-2.985976000000

Frequencies (cm⁻¹)

1	180.14
2	180.14
3	363.546
4	369.761
5	369.761
6	497.229
7	497.229
8	633.578
9	760.924

10	760.924
11	776.529
12	1320.293

[NpPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.326323000000
O	-1.394405000000	0.000000000000	-1.205353000000
O	0.697203000000	1.207590000000	-1.205353000000
O	0.697203000000	-1.207590000000	-1.205353000000
O	0.000000000000	0.000000000000	1.144856000000
Np	0.000000000000	0.000000000000	-2.862704000000

Frequencies (cm⁻¹)

1	174.182
2	174.182
3	359.631
4	367.194
5	367.194
6	493.701
7	493.701
8	628.587
9	760.294
10	760.294
11	778.478
12	1318.018

[PuPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.259051000000
O	-1.391917000000	0.000000000000	-1.135593000000
O	0.695959000000	1.205436000000	-1.135593000000
O	0.695959000000	-1.205436000000	-1.135593000000
O	0.000000000000	0.000000000000	1.213529000000
Pu	0.000000000000	0.000000000000	-2.795734000000

Frequencies (cm⁻¹)

1	180.2
2	180.2
3	357.884
4	385.606
5	385.606
6	516.764
7	516.764
8	621.663
9	763.81
10	763.81
11	786.585
12	1311.376

[AmPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.453938000000
O	-1.396405000000	0.000000000000	-1.318471000000
O	0.698203000000	1.209323000000	-1.318471000000
O	0.698203000000	-1.209323000000	-1.318471000000
O	0.000000000000	0.000000000000	1.020550000000
Am	0.000000000000	0.000000000000	-2.991968000000

Frequencies (cm⁻¹)

1	209.546
2	209.546
3	360.533
4	393.493
5	393.493
6	504.226
7	504.226
8	625.975
9	779.813
10	779.813
11	792.332
12	1309.26

[CmPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.478374000000
O	-1.402654000000	0.000000000000	-1.346222000000
O	0.701327000000	1.214734000000	-1.346222000000
O	0.701327000000	-1.214734000000	-1.346222000000
O	0.000000000000	0.000000000000	0.994501000000
Cm	0.000000000000	0.000000000000	-2.989759000000

Frequencies (cm⁻¹)

1	181.765
2	181.765
3	363.759
4	375.797
5	375.797
6	493.005
7	493.005
8	630.167
9	753.168
10	753.168
11	776.139
12	1310.336

[BkPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.465851000000
O	-1.403971000000	0.000000000000	-1.330415000000
O	0.701985000000	1.215874000000	-1.330415000000
O	0.701985000000	-1.215874000000	-1.330415000000
O	0.000000000000	0.000000000000	1.007470000000
Bk	0.000000000000	0.000000000000	-2.957216000000

Frequencies (cm⁻¹)

1	184.804
2	184.804
3	346.143
4	376.933
5	376.933
6	486.279
7	486.279
8	622.356
9	753.078
10	753.078
11	773.972
12	1304.375

[CfPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.454015000000
O	-1.399854000000	0.000000000000	-1.314515000000
O	0.699927000000	1.212309000000	-1.314515000000
O	0.699927000000	-1.212309000000	-1.314515000000
O	0.000000000000	0.000000000000	1.021284000000
Cf	0.000000000000	0.000000000000	-2.953070000000

Frequencies (cm⁻¹)

1	186.57
2	186.57
3	335.767
4	369.574
5	369.574
6	474.464
7	474.464
8	594.262
9	751.106
10	751.106
11	784.872
12	1282.667

[EsPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.640993000000

O	-1.396351000000	0.000000000000	-1.498113000000
O	0.698175000000	1.209275000000	-1.498113000000
O	0.698175000000	-1.209275000000	-1.498113000000
O	0.000000000000	0.000000000000	0.834305000000
Es	0.000000000000	0.000000000000	-3.160617000000

Frequencies (cm⁻¹)

1	197.606
2	197.606
3	319.427
4	380.931
5	380.931
6	462.432
7	462.432
8	585.312
9	747.384
10	747.384
11	786.294
12	1283.496

[FmPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.480624000000
O	-1.393744000000	0.000000000000	-1.329778000000
O	0.696872000000	1.207018000000	-1.329778000000
O	0.696872000000	-1.207018000000	-1.329778000000
O	0.000000000000	0.000000000000	0.995711000000
Fm	0.000000000000	0.000000000000	-3.015974000000

Frequencies (cm⁻¹)

1	195.583
2	195.583
3	295.112
4	377.179
5	377.179
6	441.353
7	441.353
8	564.892
9	747.505
10	747.505
11	792.494
12	1272.111

[MdPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.411890000000
O	-1.400766000000	0.000000000000	-1.218562000000
O	0.700383000000	1.213099000000	-1.218562000000
O	0.700383000000	-1.213099000000	-1.218562000000

O	0.000000000000	0.000000000000	1.078241000000
Md	0.000000000000	0.000000000000	-2.954691000000

Frequencies (cm⁻¹)

1	179.849
2	179.849
3	276.543
4	376.602
5	376.602
6	486.596
7	744.121
8	744.121
9	810.278
10	1158.565
11	1407.898
12	1407.898

[NoPO₄]

	X	Y	Z
P	0.100119000000	0.443168000000	0.000000000000
O	-0.646953000000	-0.423285000000	1.166341000000
O	-0.646953000000	-0.423285000000	-1.166341000000
O	1.532783000000	-0.280299000000	0.000000000000
O	-0.000778000000	1.918773000000	0.000000000000
No	0.311226000000	-2.174316000000	0.000000000000

Frequencies (cm⁻¹)

1	119.901
2	151.801
3	256.145
4	273.588
5	343.392
6	393.966
7	413.58
8	546.945
9	690.647
10	767.829
11	803.316
12	1228.305

[LrPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.421162000000
O	-1.415154000000	0.000000000000	-1.287852000000
O	0.707577000000	1.225560000000	-1.287852000000
O	0.707577000000	-1.225560000000	-1.287852000000
O	0.000000000000	0.000000000000	1.052913000000
Lr	0.000000000000	0.000000000000	-2.860903000000

Frequencies (cm⁻¹)

1	210.753
2	210.753
3	370.922
4	392.383
5	392.383
6	493.65
7	493.65
8	639.905
9	730.769
10	730.769
11	765.494
12	1306.459

[AcAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.427084000000
O	-1.503838000000	0.000000000000	-1.445948000000
O	0.751919000000	1.302362000000	-1.445948000000
O	0.751919000000	-1.302362000000	-1.445948000000
O	0.000000000000	0.000000000000	1.202586000000
Ac	0.000000000000	0.000000000000	-3.168946000000

Frequencies (cm⁻¹)

1	142.139
2	142.139
3	285.088
4	311.411
5	311.411
6	370.255
7	370.255
8	541.385
9	600.184
10	600.184
11	641.712
12	951.753

[UAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.349858000000
O	-1.477853000000	0.000000000000	-1.416143000000
O	0.738927000000	1.279858000000	-1.416143000000
O	0.738927000000	-1.279858000000	-1.416143000000
O	0.000000000000	0.000000000000	1.276130000000
U	0.000000000000	0.000000000000	-3.013213000000

Frequencies (cm⁻¹)

1	128.069
2	128.069
3	281.752

4	294.449
5	294.449
6	373.208
7	373.208
8	551.171
9	612.556
10	612.556
11	653.773
12	959.719

[NpAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.240478000000
O	-1.479464000000	0.000000000000	-1.303546000000
O	0.739732000000	1.281253000000	-1.303546000000
O	0.739732000000	-1.281253000000	-1.303546000000
O	0.000000000000	0.000000000000	1.387763000000
Np	0.000000000000	0.000000000000	-2.886354000000

Frequencies (cm⁻¹)

1	132.769
2	132.769
3	271.19
4	292.755
5	292.755
6	372.255
7	372.255
8	537.328
9	612.689
10	612.689
11	652.053
12	953.202

[PuAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.171592000000
O	-1.475128000000	0.000000000000	-1.232119000000
O	0.737564000000	1.277498000000	-1.232119000000
O	0.737564000000	-1.277498000000	-1.232119000000
O	0.000000000000	0.000000000000	1.457734000000
Pu	0.000000000000	0.000000000000	-2.819615000000

Frequencies (cm⁻¹)

1	139.526
2	139.526
3	274.344
4	304.864
5	304.864
6	375.653

7	375.653
8	538.637
9	616.056
10	616.056
11	661.175
12	951.69

[AmAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.367639000000
O	-1.481324000000	0.000000000000	-1.418975000000
O	0.740662000000	1.282864000000	-1.418975000000
O	0.740662000000	-1.282864000000	-1.418975000000
O	0.000000000000	0.000000000000	1.261666000000
Am	0.000000000000	0.000000000000	-3.014581000000

Frequencies (cm⁻¹)

1	158.059
2	158.059
3	278.395
4	325.727
5	325.727
6	379.331
7	379.331
8	541.869
9	624.437
10	624.437
11	661.964
12	952.464

[CmAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.396153000000
O	-1.489665000000	0.000000000000	-1.443834000000
O	0.744833000000	1.290088000000	-1.443834000000
O	0.744833000000	-1.290088000000	-1.443834000000
O	0.000000000000	0.000000000000	1.231769000000
Cm	0.000000000000	0.000000000000	-3.014996000000

Frequencies (cm⁻¹)

1	140.567
2	140.567
3	280.604
4	305.714
5	305.714
6	369.698
7	369.698
8	545.258
9	611.951

10 611.951
 11 655.525
 12 955.348

[BkAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.383001000000
O	-1.491782000000	0.000000000000	-1.429124000000
O	0.745891000000	1.291921000000	-1.429124000000
O	0.745891000000	-1.291921000000	-1.429124000000
O	0.000000000000	0.000000000000	1.244926000000
Bk	0.000000000000	0.000000000000	-2.978547000000

Frequencies (cm⁻¹)

1 142.198
 2 142.198
 3 269.049
 4 305.966
 5 305.966
 6 365.755
 7 365.755
 8 540.073
 9 612.579
 10 612.579
 11 653.595
 12 954.601

[CfAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.360504000000
O	-1.482991000000	0.000000000000	-1.410643000000
O	0.741496000000	1.284308000000	-1.410643000000
O	0.741496000000	-1.284308000000	-1.410643000000
O	0.000000000000	0.000000000000	1.269536000000
Cf	0.000000000000	0.000000000000	-2.978425000000

Frequencies (cm⁻¹)

1 163.075
 2 163.075
 3 268.576
 4 316.587
 5 316.587
 6 366.721
 7 366.721
 8 521.573
 9 607.776
 10 607.776
 11 661.139
 12 949.986

[EsAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.558785000000
O	-1.484467000000	0.000000000000	-1.605408000000
O	0.742233000000	1.285586000000	-1.605408000000
O	0.742233000000	-1.285586000000	-1.605408000000
O	0.000000000000	0.000000000000	1.070812000000
Es	0.000000000000	0.000000000000	-3.179639000000

Frequencies (cm⁻¹)

1	159.924
2	159.924
3	257.648
4	306.618
5	306.618
6	358.446
7	358.446
8	508.422
9	599.688
10	599.688
11	653.267
12	949.781

[FmAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.397491000000
O	-1.480395000000	0.000000000000	-1.438568000000
O	0.740197000000	1.282060000000	-1.438568000000
O	0.740197000000	-1.282060000000	-1.438568000000
O	0.000000000000	0.000000000000	1.232750000000
Fm	0.000000000000	0.000000000000	-3.034649000000

Frequencies (cm⁻¹)

1	159.309
2	159.309
3	242.231
4	300.917
5	300.917
6	343.493
7	343.493
8	491.455
9	589.793
10	589.793
11	657.401
12	948.692

[MdAsO₄]

X	Y	Z
---	---	---

As	0.000000000000	0.000000000000	-0.332590000000
O	-1.489700000000	0.000000000000	-1.347002000000
O	0.744850000000	1.290118000000	-1.347002000000
O	0.744850000000	-1.290118000000	-1.347002000000
O	0.000000000000	0.000000000000	1.298441000000
Md	0.000000000000	0.000000000000	-3.009051000000

Frequencies (cm⁻¹)

1	142.376
2	142.376
3	222.613
4	314.03
5	314.03
6	426.793
7	580.095
8	580.095
9	655.601
10	745.757
11	745.757
12	923.583

[NoAsO₄]

	X	Y	Z
As	0.118521000000	0.526166000000	0.000000000000
O	-0.741910000000	-0.542754000000	1.197756000000
O	-0.741910000000	-0.542754000000	-1.197756000000
O	1.641128000000	-0.349266000000	0.000000000000
O	-0.029311000000	2.151298000000	0.000000000000
No	0.312702000000	-2.193670000000	0.000000000000

Frequencies (cm⁻¹)

1	145.309
2	147.776
3	199.491
4	217.239
5	277.392
6	314.044
7	336.035
8	454.557
9	510.204
10	610.07
11	676.621
12	942.175

[LrAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.335779000000
O	-1.502753000000	0.000000000000	-1.385101000000
O	0.751377000000	1.301422000000	-1.385101000000
O	0.751377000000	-1.301422000000	-1.385101000000

O	0.000000000000	0.000000000000	1.292168000000
Lr	0.000000000000	0.000000000000	-2.882278000000

Frequencies (cm⁻¹)

1	165.018
2	165.018
3	288.302
4	329.416
5	329.416
6	371.123
7	371.123
8	541.142
9	606.386
10	606.386
11	657.853
12	954.117

Cartesian Coordinates (Angstroms) of Optimized Geometries (SO)

[AcF₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	-0.356729000000
F	-1.036568000000	-1.795388000000	0.348711000000
F	2.073136000000	0.000000000000	0.348711000000
F	-1.036568000000	1.795388000000	0.348711000000

[ThF₃]

	X	Y	Z
Th	-0.515143000000	0.474377000000	0.103253000000
F	0.190661000000	-1.083261000000	-1.118593000000
F	-2.429714000000	1.278342000000	-0.221423000000
F	0.652697000000	1.159628000000	1.710696000000

[PaF₃]

	X	Y	Z
Pa	-0.442581000000	0.594330000000	-0.003641000000
F	-0.116400000000	-1.335242000000	-0.657879000000
F	-2.487935000000	0.804951000000	0.164549000000
F	0.302255000000	0.705739000000	1.915163000000

[UF₃]

	X	Y	Z
U	-0.524738000000	0.561847000000	-0.567199000000
F	-2.352663000000	-0.296662000000	-0.170829000000
F	0.754913000000	-0.833204000000	0.241797000000
F	-0.313395000000	0.267016000000	-2.595003000000

[NpF₃]

	X	Y	Z
Np	-0.719035000000	-1.032643000000	0.086792000000
F	-2.484552000000	-2.066417000000	-0.152826000000
F	0.689369000000	-2.516374000000	-0.154425000000
F	-0.671026000000	-0.704473000000	2.120093000000

[PuF₃]

	X	Y	Z
Pu	-1.237476000000	-0.075693000000	0.246792000000
F	-1.503266000000	-2.012186000000	-0.418696000000
F	0.107517000000	0.810628000000	-1.044454000000
F	-3.042656000000	0.889905000000	-0.036691000000

[AmF₃]

	X	Y	Z
Am	-0.493623000000	-0.032977000000	0.051560000000
F	0.669101000000	-1.686415000000	-0.368379000000
F	-2.093208000000	-0.687528000000	1.187735000000
F	0.633166000000	1.204606000000	1.267082000000

[CmF₃]

	X	Y	Z
Cm	-0.649021000000	-0.479265000000	-0.720772000000
F	-2.483457000000	-1.073344000000	0.002841000000
F	0.726062000000	-1.745973000000	0.143118000000
F	-0.660706000000	-0.951995000000	-2.725383000000

[BkF₃]

	X	Y	Z
Bk	0.055064000000	0.097512000000	-0.131878000000
F	-1.670687000000	0.976227000000	0.521290000000
F	-0.438308000000	-1.854457000000	-0.479148000000
F	1.232022000000	0.061044000000	1.539184000000

[CfF₃]

	X	Y	Z
Cf	0.031991000000	0.072957000000	-0.084774000000
F	-1.696574000000	1.029403000000	0.444340000000
F	-0.425740000000	-1.862684000000	-0.557373000000
F	1.320527000000	0.091162000000	1.502330000000

[EsF₃]

	X	Y	Z
Es	-0.486284000000	-0.036169000000	-0.118589000000
F	-1.788444000000	1.500058000000	0.237367000000
F	0.147162000000	0.007164000000	-2.056827000000
F	-1.382877000000	-1.825113000000	0.302961000000

[FmF₃]

	X	Y	Z
Fm	0.100874000000	0.019725000000	-0.182165000000
F	-1.829402000000	0.414120000000	0.330787000000
F	0.196048000000	-1.950304000000	-0.691542000000
F	1.253072000000	0.281099000000	1.480521000000

[MdF₃]

	X	Y	Z
Md	-0.430015000000	0.072282000000	0.403923000000
F	-1.421363000000	1.871084000000	0.314544000000
F	-0.260369000000	-1.025760000000	-1.317906000000
F	-1.072754000000	-1.196107000000	1.870778000000

[LrF₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	-0.053137000000
F	-0.946098000000	1.638690000000	0.640528000000
F	-0.946098000000	-1.638690000000	0.640528000000
F	1.892196000000	0.000000000000	0.640528000000

[AcCl₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	-0.358249000000
Cl	-1.282533000000	-2.221413000000	0.362581000000
Cl	2.565067000000	0.000000000000	0.362581000000
Cl	-1.282533000000	2.221413000000	0.362581000000

[ThCl₃]

	X	Y	Z
Th	0.144828000000	-0.581069000000	-0.512628000000
Cl	0.209754000000	-3.126251000000	-0.277464000000
Cl	-2.088389000000	0.607977000000	-0.880905000000
Cl	2.313931000000	0.767059000000	-0.397414000000

[PaCl₃]

	X	Y	Z
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Pa	-0.449730000000	0.583083000000	0.006583000000
Cl	0.059498000000	-1.693797000000	-0.952434000000
Cl	-2.935221000000	1.006528000000	0.075920000000
Cl	0.588898000000	0.873911000000	2.286319000000

[UCl₃]

	X	Y	Z
U	-0.526402000000	0.551416000000	-0.569568000000
Cl	-2.805166000000	-0.357993000000	-0.036665000000
Cl	1.112930000000	-1.034910000000	0.478249000000
Cl	-0.239884000000	0.325579000000	-3.053498000000

[NpCl₃]

	X	Y	Z
Np	-0.720880000000	-1.044707000000	0.095760000000
Cl	-2.914151000000	-2.189936000000	-0.312716000000
Cl	1.066837000000	-2.753242000000	-0.312728000000
Cl	-0.637872000000	-0.483623000000	2.536555000000

[PuCl₃]

	X	Y	Z
Pu	-1.239550000000	-0.076730000000	0.236832000000
Cl	-1.526961000000	-2.468829000000	-0.436718000000
Cl	0.469754000000	1.032673000000	-1.213003000000
Cl	-3.424994000000	1.123997000000	0.031735000000

[AmCl₃]

	X	Y	Z
Am	-0.478112000000	-0.059597000000	0.149837000000
Cl	0.902217000000	-2.012058000000	-0.571855000000
Cl	-2.566956000000	-0.904784000000	1.253372000000
Cl	0.999280000000	1.570808000000	1.356001000000

[CmCl₃]

	X	Y	Z
Cm	-0.649048000000	-0.479358000000	-0.720719000000
Cl	-2.879251000000	-1.072900000000	0.193892000000
Cl	1.071409000000	-1.900902000000	0.366449000000
Cl	-0.635677000000	-0.924173000000	-3.163291000000

[BkCl₃]

	X	Y	Z
Bk	0.054915000000	0.095690000000	-0.131048000000

Cl	-2.019176000000	1.243967000000	0.551507000000
Cl	-0.498737000000	-2.245828000000	-0.675361000000
Cl	1.576362000000	0.117181000000	1.813466000000

[CfCl₃]

	X	Y	Z
Cf	0.020172000000	0.056322000000	-0.059327000000
Cl	-2.035103000000	1.329760000000	0.457644000000
Cl	-0.470930000000	-2.252262000000	-0.793470000000
Cl	1.673541000000	0.168218000000	1.773469000000

[EsCl₃]

	X	Y	Z
Es	-0.530648000000	-0.042545000000	-0.158728000000
Cl	-1.933140000000	1.888993000000	0.487159000000
Cl	0.514553000000	0.045826000000	-2.398232000000
Cl	-1.431286000000	-2.228173000000	0.567644000000

[FmCl₃]

	X	Y	Z
Fm	0.008352000000	0.042231000000	-0.034056000000
Cl	-2.048381000000	1.332581000000	0.448124000000
Cl	-0.482596000000	-2.258053000000	-0.811057000000
Cl	1.703590000000	0.186567000000	1.767186000000

[MdCl₃]

	X	Y	Z
Md	-0.075074000000	-0.038162000000	0.109145000000
Cl	-1.932091000000	1.627570000000	0.091824000000
Cl	-0.259064000000	-2.149300000000	-1.207938000000
Cl	1.982924000000	0.380099000000	1.456756000000

[NoCl₃]

	X	Y	Z
No	-0.051796000000	-0.016654000000	0.069804000000
Cl	-2.001022000000	1.587376000000	0.184202000000
Cl	-0.324417000000	-2.222658000000	-1.132653000000
Cl	1.950825000000	0.340780000000	1.569300000000

[LrCl₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	-0.057065000000
Cl	-1.168644000000	2.024150000000	0.605204000000

Cl	-1.168644000000	-2.024150000000	0.605204000000
Cl	2.337287000000	0.000000000000	0.605204000000

[AcBr₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	0.389759000000
Br	-1.366396000000	-2.366667000000	1.105348000000
Br	2.732792000000	0.000000000000	1.105348000000
Br	-1.366396000000	2.366667000000	1.105348000000

[ThBr₃]

	X	Y	Z
Th	-0.697363000000	-1.029091000000	0.063315000000
Br	-3.319134000000	-1.662617000000	0.347286000000
Br	0.598031000000	-1.618220000000	-2.245458000000
Br	0.629661000000	0.191303000000	2.089432000000

[PaBr₃]

	X	Y	Z
Pa	-0.482335000000	0.531327000000	0.052660000000
Br	0.135747000000	-1.827850000000	-1.071348000000
Br	-3.108542000000	1.093764000000	0.035639000000
Br	0.706969000000	0.943838000000	2.425262000000

[UBr₃]

	X	Y	Z
U	-0.532731000000	0.503233000000	-0.585115000000
Br	-2.986246000000	-0.376444000000	0.021225000000
Br	1.257394000000	-1.109859000000	0.578695000000
Br	-0.209798000000	0.358478000000	-3.237393000000

[NpBr₃]

	X	Y	Z
Np	-0.724056000000	-1.072227000000	0.120006000000
Br	-3.067075000000	-2.248706000000	-0.367284000000
Br	1.198589000000	-2.854041000000	-0.369940000000
Br	-0.628900000000	-0.408013000000	2.698069000000

[PuBr₃]

	X	Y	Z
Pu	-1.249833000000	-0.078472000000	0.201833000000
Br	-1.538040000000	-2.638340000000	-0.461717000000
Br	0.600275000000	1.110894000000	-1.293052000000

Br	-3.572054000000	1.209996000000	0.042356000000
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[AmBr₃]

	X	Y	Z
Am	-0.381722000000	-1.549128000000	-0.353671000000
Br	-0.935692000000	-1.185923000000	-2.939270000000
Br	2.237606000000	-1.442973000000	0.137417000000
Br	-1.705740000000	-3.669175000000	0.574742000000

[CmBr₃]

	X	Y	Z
Cm	-0.664494000000	-0.554199000000	-0.733626000000
Br	-3.042898000000	-1.114264000000	0.260830000000
Br	1.198482000000	-2.003347000000	0.444704000000
Br	-0.633403000000	-0.955835000000	-3.341440000000

[BkBr₃]

	X	Y	Z
Bk	0.024235000000	0.058699000000	-0.072504000000
Br	-2.173157000000	1.330922000000	0.593655000000
Br	-0.540670000000	-2.420705000000	-0.722856000000
Br	1.696750000000	0.121771000000	1.953403000000

[CfBr₃]

	X	Y	Z
Cf	-0.070474000000	-0.051313000000	0.110027000000
Br	-2.213423000000	1.416107000000	0.554828000000
Br	-0.533531000000	-2.473138000000	-0.824562000000
Br	1.790809000000	0.177902000000	1.963565000000

[EsBr₃]

	X	Y	Z
Es	-1.033967000000	-0.029211000000	-0.130251000000
Br	-1.945548000000	2.156499000000	1.033704000000
Br	-0.416597000000	0.025529000000	-2.695200000000
Br	-1.848994000000	-2.300604000000	0.934238000000

[FmBr₃]

	X	Y	Z
Fm	-0.043314000000	-0.013810000000	0.056066000000
Br	-2.226150000000	1.368531000000	0.597345000000
Br	-0.549272000000	-2.478119000000	-0.748543000000
Br	1.746209000000	0.126085000000	1.991588000000

[MdBr₃]

	X	Y	Z
Md	0.103885000000	0.347887000000	-0.045416000000
Br	-2.319337000000	1.345902000000	0.423974000000
Br	0.856041000000	-0.169488000000	-2.555386000000
Br	1.899122000000	0.015217000000	1.901028000000

[NoBr₃]

	X	Y	Z
No	-0.128775000000	-0.139549000000	-0.585538000000
Br	-2.295003000000	1.359908000000	-0.027025000000
Br	-0.342928000000	-2.823824000000	-0.619970000000
Br	2.084639000000	1.033316000000	-1.574717000000

[LrBr₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	0.080273000000
Br	-1.258908000000	2.180492000000	0.649819000000
Br	-1.258908000000	-2.180492000000	0.649819000000
Br	2.517816000000	0.000000000000	0.649819000000

[AcI₃]

	X	Y	Z
Ac	0.000000000000	0.000000000000	0.465259000000
I	-1.482379000000	-2.567556000000	1.188478000000
I	2.964758000000	0.000000000000	1.188478000000
I	-1.482379000000	2.567556000000	1.188478000000

[ThI₃]

	X	Y	Z
Th	-0.697086000000	-1.029960000000	0.063726000000
I	-3.536249000000	-1.715225000000	0.370668000000
I	0.705220000000	-1.667123000000	-2.436662000000
I	0.739671000000	0.292340000000	2.257287000000

[PaI₃]

	X	Y	Z
Pa	-0.513104000000	0.478730000000	0.099622000000
I	0.210415000000	-2.022803000000	-1.206667000000
I	-3.340125000000	1.176248000000	0.007668000000
I	0.836734000000	1.014771000000	2.625375000000

[U₃]

	X	Y	Z
U	-0.534420000000	0.485384000000	-0.592547000000
I	-3.203216000000	-0.435125000000	0.084344000000
I	1.419642000000	-1.234168000000	0.692716000000
I	-0.178434000000	0.368020000000	-3.470302000000

[Np₃]

	X	Y	Z
Np	-0.724713000000	-1.076633000000	0.122917000000
I	-3.278075000000	-2.316591000000	-0.434359000000
I	1.382968000000	-2.976915000000	-0.437711000000
I	-0.614727000000	-0.312096000000	2.907033000000

[Pu₃]

	X	Y	Z
Pu	-1.269600000000	-0.079700000000	0.147500000000
I	-1.542200000000	-2.891300000000	-0.476000000000
I	0.804900000000	1.225400000000	-1.389000000000
I	-3.787700000000	1.342800000000	0.083300000000

[Am₃]

	X	Y	Z
Am	-0.339556000000	-1.629778000000	-0.395464000000
I	-1.020510000000	-1.075880000000	-3.173370000000
I	2.490803000000	-1.382645000000	0.236467000000
I	-1.863257000000	-3.840476000000	0.728305000000

[Cm₃]

	X	Y	Z
Cm	-0.678142000000	-0.621515000000	-0.743512000000
I	-3.266690000000	-1.171588000000	0.348505000000
I	1.372351000000	-2.143959000000	0.550237000000
I	-0.632684000000	-1.000410000000	-3.581716000000

[Bk₃]

	X	Y	Z
Bk	-0.020185000000	0.002266000000	0.020251000000
I	-2.390414000000	1.468171000000	0.636822000000
I	-0.598848000000	-2.667161000000	-0.814439000000
I	1.885670000000	0.144603000000	2.145582000000

[Cf₃]

	X	Y	Z
Cf	-0.158615000000	-0.159467000000	0.263772000000
I	-2.444330000000	1.520602000000	0.696248000000
I	-0.619743000000	-2.772767000000	-0.833700000000
I	1.910247000000	0.165652000000	2.230608000000

[EsI₃]

	X	Y	Z
Es	-1.672311000000	-0.038110000000	-0.445409000000
I	-2.034789000000	2.275753000000	1.212657000000
I	-0.295501000000	0.039453000000	-2.978001000000
I	-1.929352000000	-2.431823000000	1.116000000000

[FmI₃]

	X	Y	Z
Fm	-0.287102000000	-0.278582000000	0.520539000000
I	-2.442047000000	1.654165000000	0.484274000000
I	-0.527855000000	-2.712057000000	-1.029395000000
I	2.096196000000	0.235483000000	2.081301000000

[MdI₃]

	X	Y	Z
Md	0.064613000000	0.196639000000	-0.036223000000
I	-2.391239000000	1.682326000000	0.446643000000
I	0.980870000000	0.051449000000	-2.794007000000
I	2.092714000000	0.265806000000	2.049367000000

[NoI₃]

	X	Y	Z
No	-0.149780000000	-0.141521000000	-0.643291000000
I	-2.482675000000	1.500631000000	0.054113000000
I	-0.350647000000	-3.071177000000	-0.593418000000
I	2.298098000000	1.142427000000	-1.635354000000

[LrI₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	0.270533000000
I	-1.385919000000	2.400482000000	0.677515000000
I	-1.385919000000	-2.400482000000	0.677515000000
I	2.771838000000	0.000000000000	0.677515000000

[AcAt₃]

	X	Y	Z
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Ac	0.000000000000	0.000000000000	0.439881000000
At	-1.531705000000	-2.652990000000	1.243252000000
At	3.063409000000	0.000000000000	1.243252000000
At	-1.531705000000	2.652990000000	1.243252000000

[ThAt₃]

	X	Y	Z
Th	-0.696367000000	-1.030994000000	0.064085000000
At	-3.646848000000	-1.741464000000	0.382468000000
At	0.759465000000	-1.691818000000	-2.534752000000
At	0.795246000000	0.344435000000	2.343163000000

[PaAt₃]

	X	Y	Z
Pa	-0.505929000000	0.493632000000	0.087349000000
At	0.234753000000	-2.120855000000	-1.249800000000
At	-3.450381000000	1.197066000000	0.007348000000
At	0.886251000000	1.028484000000	2.724457000000

[UAt₃]

	X	Y	Z
U	-0.529721000000	0.516596000000	-0.583112000000
At	-3.301004000000	-0.460517000000	0.112721000000
At	1.493381000000	-1.289409000000	0.744621000000
At	-0.164329000000	0.373249000000	-3.576001000000

[NpAt₃]

	X	Y	Z
Np	-0.727234000000	-1.095641000000	0.137486000000
At	-3.392659000000	-2.373118000000	-0.456059000000
At	1.477484000000	-3.063337000000	-0.460000000000
At	-0.610590000000	-0.281046000000	3.033035000000

[PuAt₃]

	X	Y	Z
Pu	-1.226147000000	-0.075388000000	0.281824000000
At	-1.566391000000	-2.949796000000	-0.546266000000
At	0.826035000000	1.249821000000	-1.477203000000
At	-3.854897000000	1.369256000000	0.023304000000

[AmAt₃]

	X	Y	Z
Am	-0.383882000000	-1.546025000000	-0.350219000000

At	-1.037317000000	-1.052306000000	-3.284837000000
At	2.593480000000	-1.401134000000	0.268816000000
At	-1.890318000000	-3.935044000000	0.785858000000

[CmAt₃]

	X	Y	Z
Cm	-0.678524000000	-0.622971000000	-0.742292000000
At	-3.372698000000	-1.202810000000	0.389627000000
At	1.453061000000	-2.214233000000	0.599630000000
At	-0.633135000000	-1.025489000000	-3.694582000000

[BkAt₃]

	X	Y	Z
Bk	-0.011574000000	0.012783000000	-0.003845000000
At	-2.491999000000	1.512030000000	0.691944000000
At	-0.625275000000	-2.789018000000	-0.813969000000
At	1.937526000000	0.126930000000	2.249482000000

[CfAt₃]

	X	Y	Z
Cf	-0.171009000000	-0.176052000000	0.294802000000
At	-2.593346000000	1.536240000000	0.780458000000
At	-0.683842000000	-2.928851000000	-0.803553000000
At	1.969517000000	0.122059000000	2.390342000000

[EsAt₃]

	X	Y	Z
Es	-1.427822000000	-0.036391000000	-0.282427000000
At	-2.478307000000	2.479700000000	1.003520000000
At	-0.750008000000	0.035440000000	-3.224998000000
At	-2.364847000000	-2.646527000000	0.899649000000

[FmAt₃]

	X	Y	Z
Fm	-0.315513000000	-0.314984000000	0.578557000000
At	-2.556626000000	1.723409000000	0.517812000000
At	-0.559281000000	-2.845602000000	-1.069211000000
At	2.188452000000	0.243750000000	2.190230000000

[MdAt₃]

	X	Y	Z
Md	0.077372000000	0.220383000000	-0.040959000000
At	-2.459104000000	1.827047000000	0.458350000000

At	1.047285000000	0.128524000000	-2.921931000000
At	2.204122000000	0.353926000000	2.129748000000

[NoAt₃]

	X	Y	Z
No	-0.161909000000	-0.142655000000	-0.677365000000
At	-2.589188000000	1.580315000000	0.102976000000
At	-0.354906000000	-3.212453000000	-0.575581000000
At	2.420987000000	1.204867000000	-1.667552000000

[LrAt₃]

	X	Y	Z
Lr	0.000000000000	0.000000000000	0.410146000000
At	-1.455340000000	2.520723000000	0.680377000000
At	-1.455340000000	-2.520723000000	0.680377000000
At	2.910680000000	0.000000000000	0.680377000000

[AcPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.575201000000
O	-1.407084000000	0.000000000000	-1.411244000000
O	0.703542000000	1.218570000000	-1.411244000000
O	0.703542000000	-1.218570000000	-1.411244000000
O	0.000000000000	0.000000000000	0.893828000000
Ac	0.000000000000	0.000000000000	-3.192083000000

[ThPO₄]

	X	Y	Z
P	0.152240000000	-1.186032000000	0.247439000000
O	-1.390151000000	-1.568883000000	-0.167051000000
O	0.595743000000	-0.846483000000	-1.297179000000
O	0.672580000000	-2.741906000000	0.167204000000
O	0.471304000000	-0.305781000000	1.370421000000
Th	-0.409380000000	-2.738273000000	-1.732045000000

[PaPO₄]

	X	Y	Z
P	0.136682000000	-1.231507000000	0.194327000000
O	-1.406337000000	-1.609886000000	-0.218627000000
O	0.581612000000	-0.886319000000	-1.350140000000
O	0.658715000000	-2.783569000000	0.117222000000
O	0.455791000000	-0.347635000000	1.314352000000
Pa	-0.419064000000	-2.763583000000	-1.768234000000

[UPO₄]

	X	Y	Z
P	0.135420000000	-1.232785000000	0.184833000000
O	-1.410836000000	-1.608592000000	-0.218315000000
O	0.584122000000	-0.881445000000	-1.350700000000
O	0.661319000000	-2.787731000000	0.117906000000
O	0.454320000000	-0.353465000000	1.310619000000
U	-0.416945000000	-2.758481000000	-1.755542000000

[NpPO₄]

	X	Y	Z
P	0.132348000000	-1.242430000000	0.188015000000
O	-1.412618000000	-1.609668000000	-0.215856000000
O	0.584218000000	-0.884314000000	-1.351548000000
O	0.661960000000	-2.788609000000	0.120694000000
O	0.453731000000	-0.354205000000	1.307737000000
Np	-0.412340000000	-2.743373000000	-1.760242000000

[PuPO₄]

	X	Y	Z
P	0.200015000000	-1.052928000000	0.419111000000
O	-1.344862000000	-1.419076000000	0.022320000000
O	0.652575000000	-0.695940000000	-1.115430000000
O	0.731945000000	-2.599827000000	0.358662000000
O	0.520281000000	-0.170307000000	1.544890000000
Pu	-0.347262000000	-2.565725000000	-1.513379000000

[AmPO₄]

	X	Y	Z
P	0.128456000000	-1.264680000000	0.196733000000
O	-1.417203000000	-1.586715000000	-0.199389000000
O	0.571062000000	-0.902506000000	-1.367208000000
O	0.674184000000	-2.787356000000	0.135153000000
O	0.473072000000	-0.351804000000	1.292422000000
Am	-0.422272000000	-2.729538000000	-1.768910000000

[CmPO₄]

	X	Y	Z
P	0.158920000000	-1.184909000000	0.248909000000
O	-1.395787000000	-1.541124000000	-0.131138000000
O	0.606719000000	-0.822025000000	-1.286170000000
O	0.683813000000	-2.737298000000	0.192640000000
O	0.490943000000	-0.303635000000	1.373190000000
Cm	-0.405776000000	-2.684520000000	-1.663285000000

[BkPO₄]

	X	Y	Z
P	0.138050000000	-1.241825000000	0.169804000000
O	-1.416947000000	-1.602416000000	-0.208158000000
O	0.585892000000	-0.877800000000	-1.360932000000
O	0.658975000000	-2.797286000000	0.114663000000
O	0.467882000000	-0.364602000000	1.298158000000
Bk	-0.426352000000	-2.738771000000	-1.724736000000

[CfPO₄]

	X	Y	Z
P	0.167344000000	-1.157426000000	0.257594000000
O	-1.385909000000	-1.529144000000	-0.108862000000
O	0.619103000000	-0.794281000000	-1.258075000000
O	0.681336000000	-2.720818000000	0.206599000000
O	0.496496000000	-0.292142000000	1.396978000000
Cf	-0.397914000000	-2.669832000000	-1.619677000000

[EsPO₄]

	X	Y	Z
P	0.138059000000	-1.236742000000	0.163564000000
O	-1.411221000000	-1.602539000000	-0.206134000000
O	0.588683000000	-0.873717000000	-1.354184000000
O	0.655432000000	-2.791701000000	0.112260000000
O	0.465808000000	-0.367608000000	1.300780000000
Es	-0.429162000000	-2.750492000000	-1.727387000000

[FmPO₄]

	X	Y	Z
P	0.158060000000	-1.188945000000	0.247666000000
O	-1.388972000000	-1.536479000000	-0.123856000000
O	0.606800000000	-0.820348000000	-1.274435000000
O	0.683487000000	-2.727598000000	0.199921000000
O	0.490763000000	-0.302616000000	1.370668000000
Fm	-0.406115000000	-2.684557000000	-1.668917000000

[MdPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.602388000000
O	-1.398161000000	0.000000000000	-1.419034000000
O	0.699081000000	1.210843000000	-1.419034000000
O	0.699081000000	-1.210843000000	-1.419034000000
O	0.000000000000	0.000000000000	0.874114000000

Md 0.000000000000 0.000000000000 -3.107645000000

[NoPO₄]

	X	Y	Z
P	0.097165000000	0.000000000000	0.434903000000
O	-0.627607000000	-1.171489000000	-0.433501000000
O	-0.627607000000	1.171490000000	-0.433500000000
O	1.529040000000	0.000001000000	-0.284026000000
O	-0.008173000000	0.000000000000	1.902534000000
No	0.286626000000	-0.000001000000	-2.125655000000

[LrPO₄]

	X	Y	Z
P	0.000000000000	0.000000000000	-0.427859000000
O	-1.409660000000	0.000000000000	-1.285493000000
O	0.704830000000	1.220801000000	-1.285493000000
O	0.704830000000	-1.220801000000	-1.285493000000
O	0.000000000000	0.000000000000	1.039172000000
Lr	0.000000000000	0.000000000000	-2.847542000000

[AcAsO₄]

	X	Y	Z
As	0.000000000000	0.000000000000	-0.431009000000
O	-1.503307000000	0.000000000000	-1.449728000000
O	0.751654000000	1.301902000000	-1.449728000000
O	0.751654000000	-1.301902000000	-1.449728000000
O	0.000000000000	0.000000000000	1.198962000000
Ac	0.000000000000	0.000000000000	-3.166596000000

[UAsO₄]

	X	Y	Z
As	0.179974000000	-1.108246000000	0.345295000000
O	-1.497832000000	-1.588535000000	-0.186685000000
O	0.630940000000	-0.811405000000	-1.395631000000
O	0.712452000000	-2.846640000000	0.172046000000
O	0.536248000000	-0.132370000000	1.594594000000
U	-0.395953000000	-2.700884000000	-1.684493000000

[NpAsO₄]

	X	Y	Z
As	0.204711000000	-1.039891000000	0.436160000000
O	-1.471762000000	-1.517909000000	-0.093670000000
O	0.655620000000	-0.745123000000	-1.304626000000
O	0.737895000000	-2.773880000000	0.264171000000

O	0.563966000000	-0.055681000000	1.681116000000
Np	-0.368957000000	-2.626373000000	-1.590340000000

[PuAsO₄]

	X	Y	Z
As	0.216754000000	-0.999518000000	0.484178000000
O	-1.456603000000	-1.471981000000	-0.040503000000
O	0.671032000000	-0.705454000000	-1.255040000000
O	0.754288000000	-2.730953000000	0.311622000000
O	0.580695000000	-0.024537000000	1.736487000000
Pu	-0.353641000000	-2.585156000000	-1.536846000000

[AmAsO₄]

	X	Y	Z
As	0.175684000000	-1.136976000000	0.347798000000
O	-1.502901000000	-1.566905000000	-0.168318000000
O	0.608197000000	-0.856480000000	-1.431005000000
O	0.726284000000	-2.843267000000	0.190941000000
O	0.568491000000	-0.105109000000	1.544878000000
Am	-0.410713000000	-2.698111000000	-1.689060000000

[CmAsO₄]

	X	Y	Z
As	0.177191000000	-1.133919000000	0.313123000000
O	-1.510234000000	-1.595051000000	-0.195378000000
O	0.624563000000	-0.828569000000	-1.426717000000
O	0.706828000000	-2.870270000000	0.149785000000
O	0.548904000000	-0.157953000000	1.561962000000
Cm	-0.412804000000	-2.703482000000	-1.687612000000

[BkAsO₄]

	X	Y	Z
As	0.181282000000	-1.123179000000	0.324638000000
O	-1.505609000000	-1.586219000000	-0.182483000000
O	0.629353000000	-0.815658000000	-1.413497000000
O	0.708251000000	-2.860283000000	0.161840000000
O	0.552085000000	-0.150734000000	1.576455000000
Bk	-0.404883000000	-2.682750000000	-1.660633000000

[CfAsO₄]

	X	Y	Z
As	0.185265000000	-1.105787000000	0.329361000000
O	-1.496880000000	-1.583030000000	-0.173226000000
O	0.637547000000	-0.797156000000	-1.390100000000

O	0.699530000000	-2.853835000000	0.155530000000
O	0.554908000000	-0.159148000000	1.602998000000
Cf	-0.404103000000	-2.682065000000	-1.656257000000

[EsAsO₄]

	X	Y	Z
As	0.141638000000	-1.224630000000	0.181231000000
O	-1.538594000000	-1.695309000000	-0.322457000000
O	0.593882000000	-0.915158000000	-1.540299000000
O	0.661261000000	-2.965394000000	0.010316000000
O	0.505382000000	-0.273244000000	1.452987000000
Es	-0.449354000000	-2.804113000000	-1.811295000000

[FmAsO₄]

	X	Y	Z
As	0.175406000000	-1.138670000000	0.309970000000
O	-1.504178000000	-1.596941000000	-0.192770000000
O	0.622980000000	-0.832722000000	-1.418652000000
O	0.702980000000	-2.864677000000	0.151285000000
O	0.549706000000	-0.154915000000	1.553652000000
Fm	-0.416364000000	-2.713780000000	-1.701719000000

[MdAsO₄]

	X	Y	Z
As	0.189610000000	-1.100091000000	0.345719000000
O	-1.491403000000	-1.590714000000	-0.105402000000
O	0.645368000000	-0.793036000000	-1.366419000000
O	0.686510000000	-2.839618000000	0.226332000000
O	0.566373000000	-0.117337000000	1.591530000000
Md	-0.407840000000	-2.692348000000	-1.677532000000

[NoAsO₄]

	X	Y	Z
As	0.113514000000	-0.000005000000	0.508691000000
O	-0.708360000000	-1.219319000000	-0.565123000000
O	-0.708348000000	1.219312000000	-0.565128000000
O	1.645153000000	0.000000000000	-0.370065000000
O	-0.032199000000	0.000016000000	2.133278000000
No	0.309936000000	0.000001000000	-2.183455000000

[LrAsO₄]

	X	Y	Z
As	0.191138000000	-1.096312000000	0.361199000000
O	-1.508745000000	-1.558160000000	-0.147838000000

O	0.643985000000	-0.785302000000	-1.388584000000
O	0.726651000000	-2.843603000000	0.200733000000
O	0.562388000000	-0.121014000000	1.609267000000
Lr	-0.382511000000	-2.624299000000	-1.586791000000