Theoretical Studies of Cyclic Adenosine Monophosphate Dependent Protein Kinase: Native Enzyme and Ground-State and Transition-State Analogues

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Supporting Information
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Model Details

An unpublished, 2.0 Å resolution, disordered X-ray crystal structure (analogous to PDB ID: 1L3R)[1] containing a twenty-residue peptide substrate as well as MgF_3^- and AlF_4^- transition-state analogues was used to create a computational model of the cAPK enzyme. This 339-atom model (340 atoms for AlF_4^-) included twenty-four residues of the active site, two Mg^{2+} cofactors, the transition-state analogue species, and five residues of the peptide substrate (see Table S1 and Figures S1 and S2). The active-site species (YX_n) was varied to be PO_3^-, BeF_3^-, MgF_3^-, AlF_4^-, and AlF_3^0. Residues on the outermost part of the model were capped with hydrogen atoms. The R-groups of several residues and the adenine of ATP were also trimmed and capped with hydrogens. The model has an overall charge of 1+ when a monoanion species is in the active site and 2+ when the neutral AlF_3 is in the active site.

Table S1. Complete and truncated residues included in the computational model.

Complete residue		Backbone only
ARG18[a]	GLY186	ARG19[a]
SER21[a]	PHE187	ALA20[a]
GLY50	GLY200	ILE22[a]
GLY52	THR201	THR51
SER53	MGF3	LEU167
PHE54	MG391	GLU170
GLY55	MG392	PHE185
LYS72	HOH426	
ASP166	HOH444	ADP381; no adenine
LYS168	HOH576	
PRO169	HOH577	
ASN171	HOH578	
ASP184		

[a]Residue belongs to peptide substrate

Table S2. Details of the geometric constraints of the model.

non-constrained	partially constrained–non-constrained[b]	constrained
GLY52	ALA20[a]–backbone carbonyl	ARG18[a]
MG391	SER21[a]–R-group, backbone amine, α-carbon	ARG19[a]
MG392	SER53–backbone	ILE22[a]
AlF4: AL620	PHE54–backbone	GLY50
AlF4: F1, F2, F3, F4	GLY55–backbone amine, α-carbon	THR51
YF3: MG5144/Al	LYS72–part of R-group	LEU167
YF3: F1, F2, F3	ASP166–R-group	PRO169
HOH426	LYS168–part of R-group	GLU170
HOH444	ASN171–R-group	PHE185
HOH576	ASP184–R-group	GLY186
HOH577	ADP381–phosphoryl groups	PHE187
HOH578		GLY200
		THR201

[a]Residue belongs to peptide substrate [b]Non-constrained portion of a partially constrained residue/nucleoside

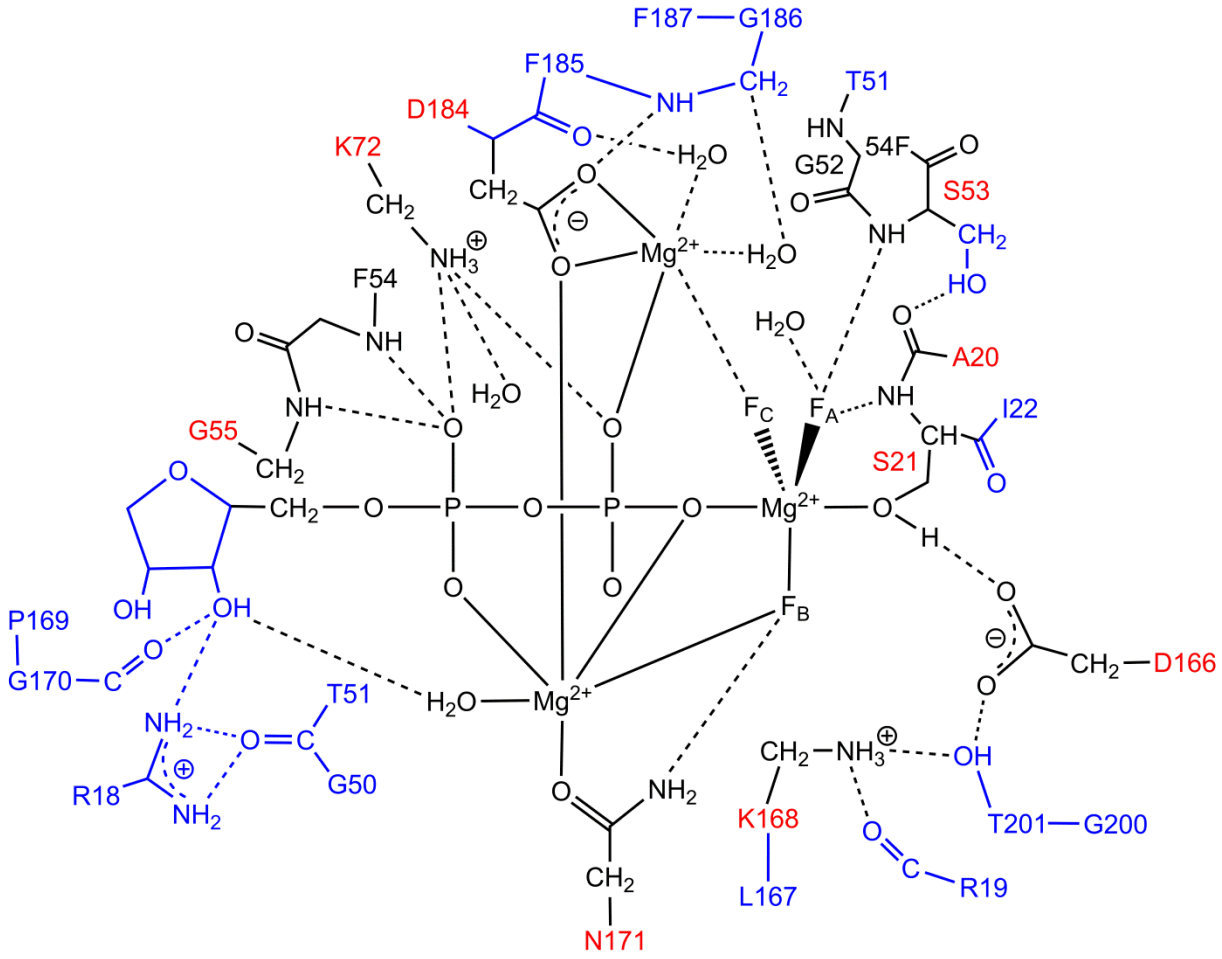


Figure S1. A 2D-representation of the 339-atom model of the MgF_3–TSA of cAPK. Residues in which select atoms are constrained are in red; constrained atoms are in blue; and non-constrained atoms are in black. Hydrogen bonds are indicated by dashed lines.

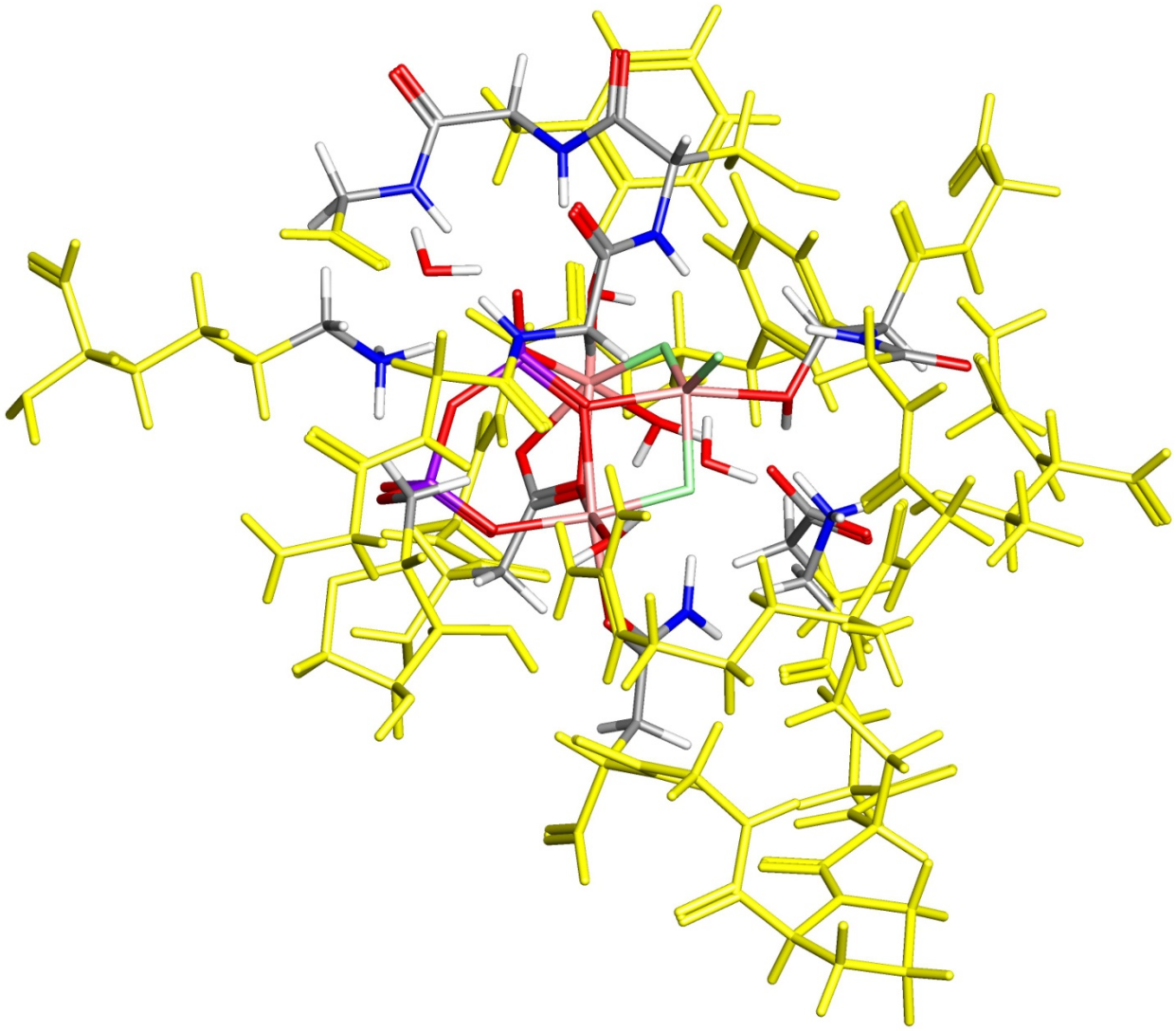


Figure S2. A 3D-representation of the 339-atom model of the MgF_3–TSA of cAPK. Atoms in yellow were constrained to their crystallographically-determined positions. Atoms in standard colors were allowed to freely optimize.

Computational Details

Except where noted, all computations were performed with Gaussian 09.B01.[2] Geometries were optimized using the B3LYP functional (the Becke three-parameter functional[3] and the Lee-Yang-Parr gradient-corrected correlation functional[4]) of Density Functional Theory (DFT).[5] The substrate and the surrounding atoms involved in hydrogen bonding were allowed to freely optimize (102 atoms). The remaining 237 atoms were geometrically constrained to their crystallographically-determined locations to provide a support for the non-constrained atoms (Table S2). The large number of constrained atoms is due to the inclusion of many R-groups not directly involved in the mechanism. To our knowledge, this 339-atom model (102 non-constrained atoms) represents the largest cAPK model treated quantum mechanically (with DFT) to date. The 102 non-constrained atoms were treated with the 6-31G(d') basis sets[6, 7] (which for Mg, Al, and P are the same basis sets as 6-31G(d) but for the other atoms have the *d* polarization functions taken from the 6-311G(d) basis sets,[8] rather than the default value of 0.8 used in the 6-31G(d) basis sets). The remaining 237 atoms were treated with the 6-31G basis sets.[9] This combination of basis sets is referred to as BS1. Except where noted, each optimized geometry was verified to be a zeroth- or first-order saddle point by an analytical frequency calculation.

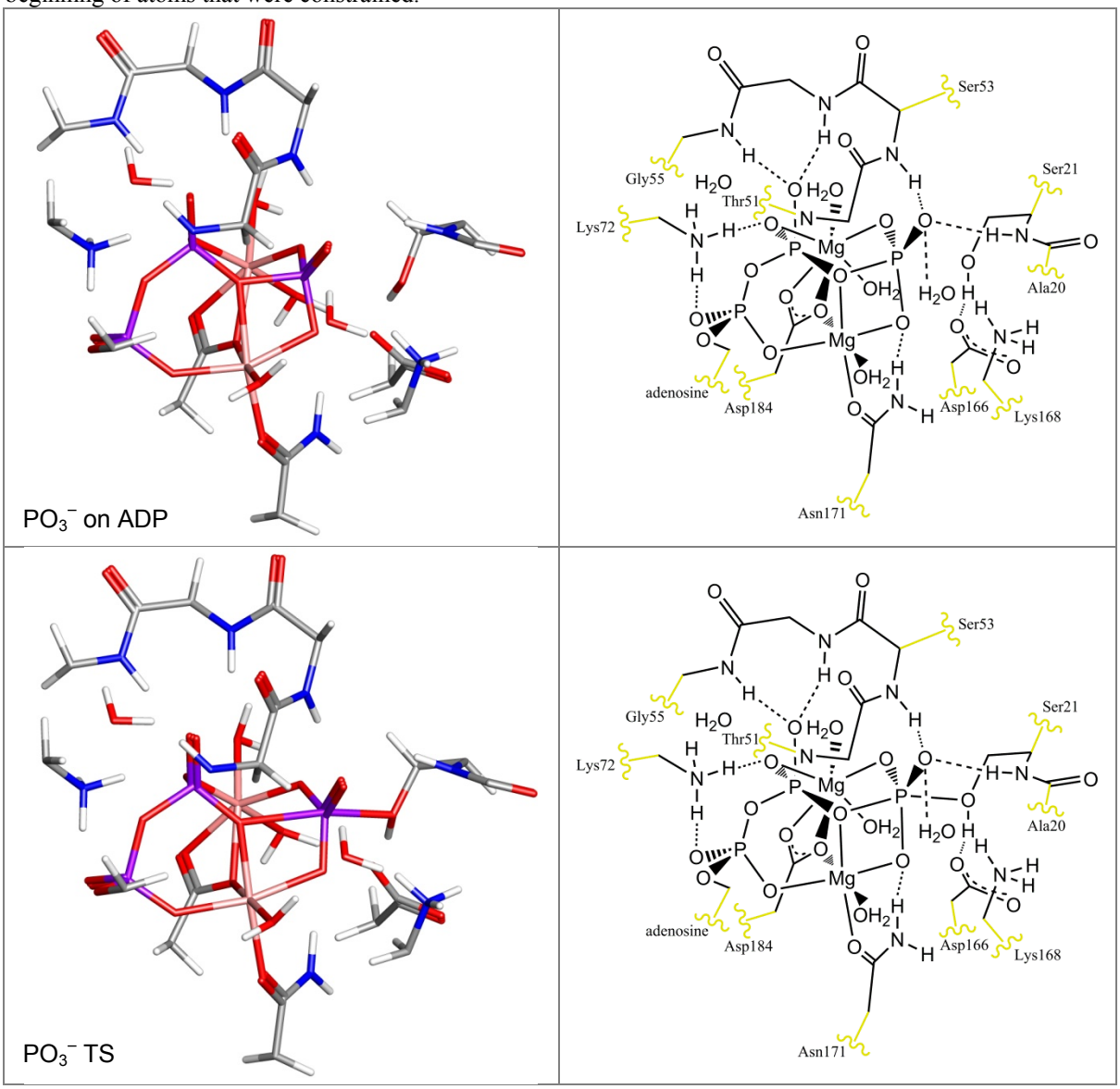
To simulate the protein environment, B3LYP single-point calculations were performed on the gas-phase DFT optimized geometries using the COSMO polarizable conductor model (CPCM).[10] The UAKS (United Atom Kohn-Sham) atomic radii,[10] a non-default electrostatic scaling factor of 1.2, and a dielectric constant of 4.0 were used.[11] Optimizations with CPCM were also performed on the three PO_3-containing stationary points for comparison.

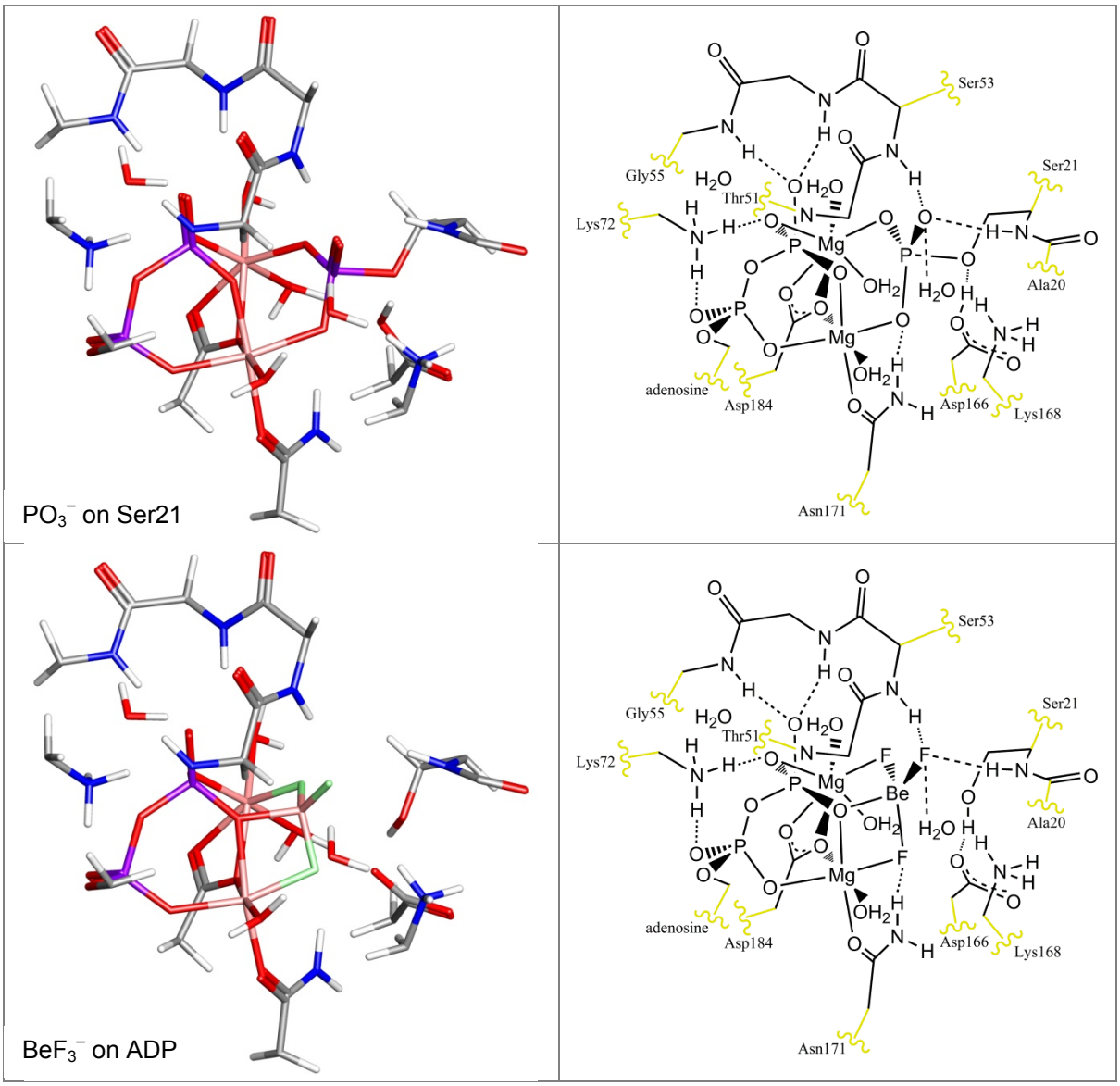
An additional B3LYP single-point calculation was used to compute the absolute isotropic shielding values under solvated conditions (in ppm). Within the non-constrained atoms, Mg, Al, Be, and P atoms utilized the 6-311G(2d,2p) basis sets,[8] and the remaining non-constrained atoms utilized the EPR-II basis sets.[12] (IGLO-II basis sets gave similar results.) The frozen atoms utilized the STO-3G basis set.[13] The computed chemical shifts are referenced to gas-phase computations of the fluorine absolute isotropic shielding value for $CFCl_3$ (gas-phase absolute isotropic shielding of 171.3531 ppm). The simulated NMR spectra were produced with an in-house program using Gaussian broadening of 0.5 ppm.

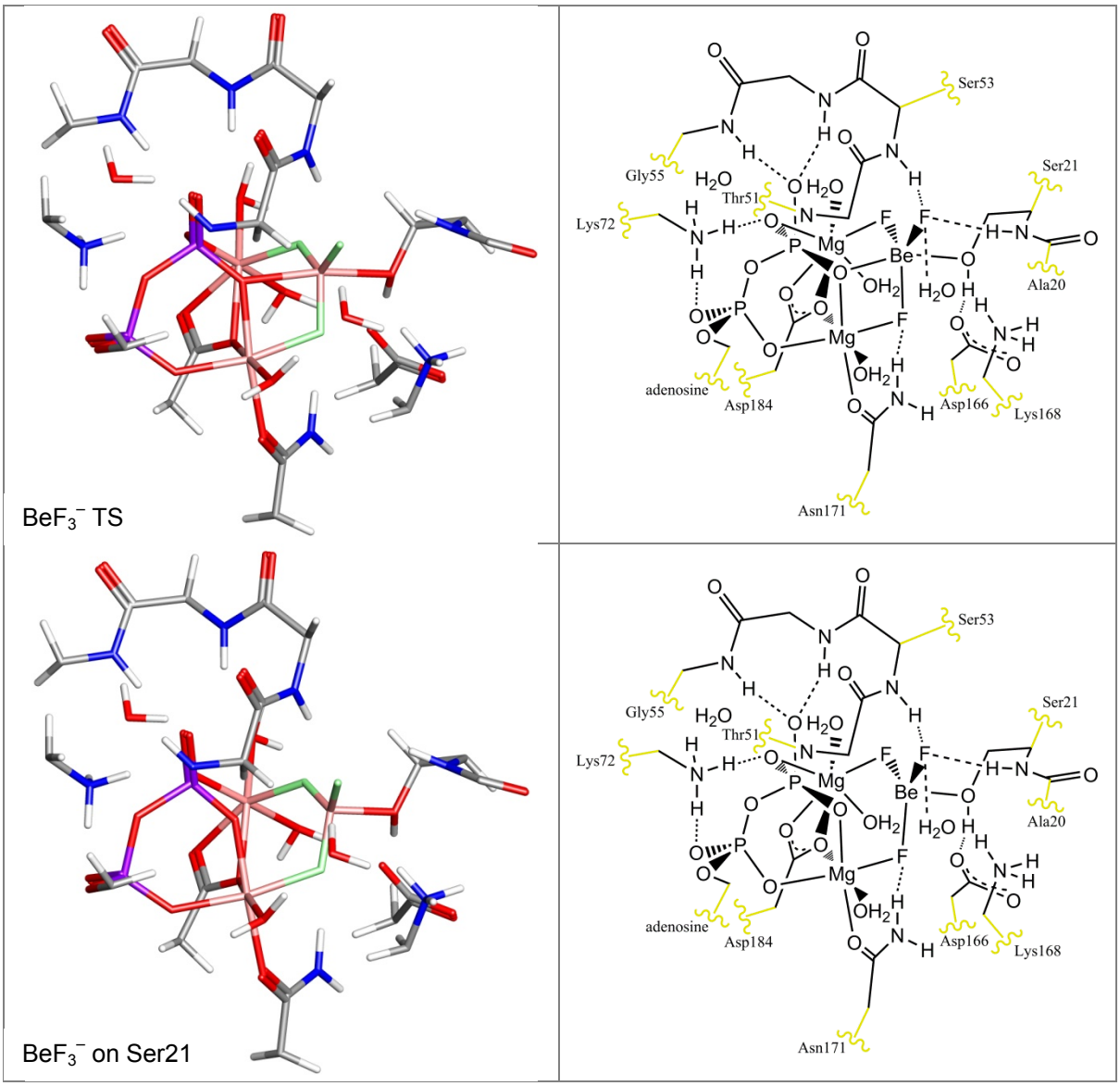
To test the basis set dependency, B3LYP geometry optimizations were also performed using the 6-31+G(d',p')[6, 7, 14] basis sets on the non-constrained atoms (referred to as BS2). To examine the effects of dispersion, the geometries were also optimized with B3LYP and GD3BJ dispersion (Grimme's D3 dispersion with Becke-Johnson damping[15] [referred to "B3LYP-D"] using Gaussian 09.D01[16]) and the ωB97xD[17] functional. BS1 was used for the B3LYP-D and ωB97xD computations.

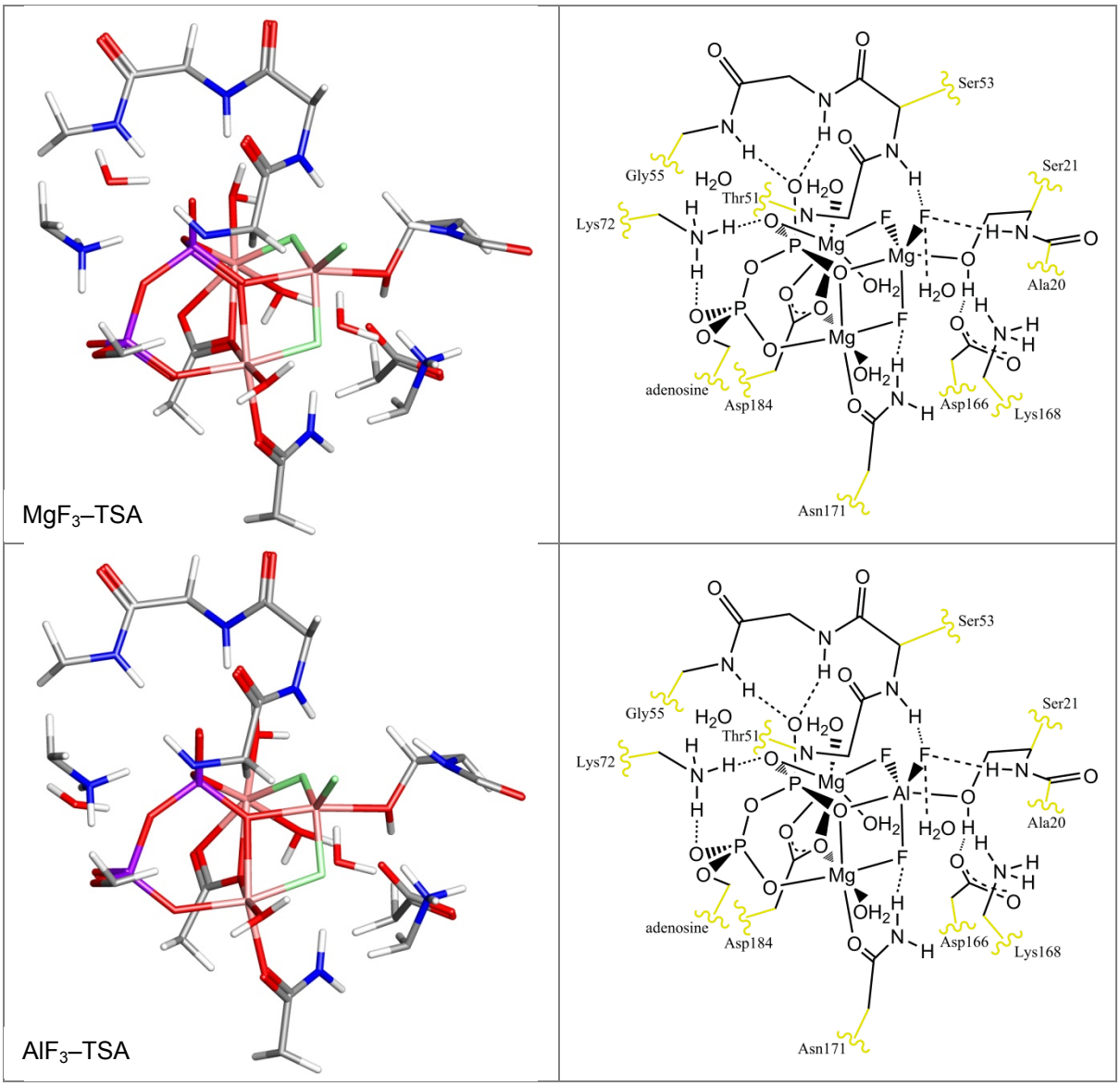
Optimized geometries

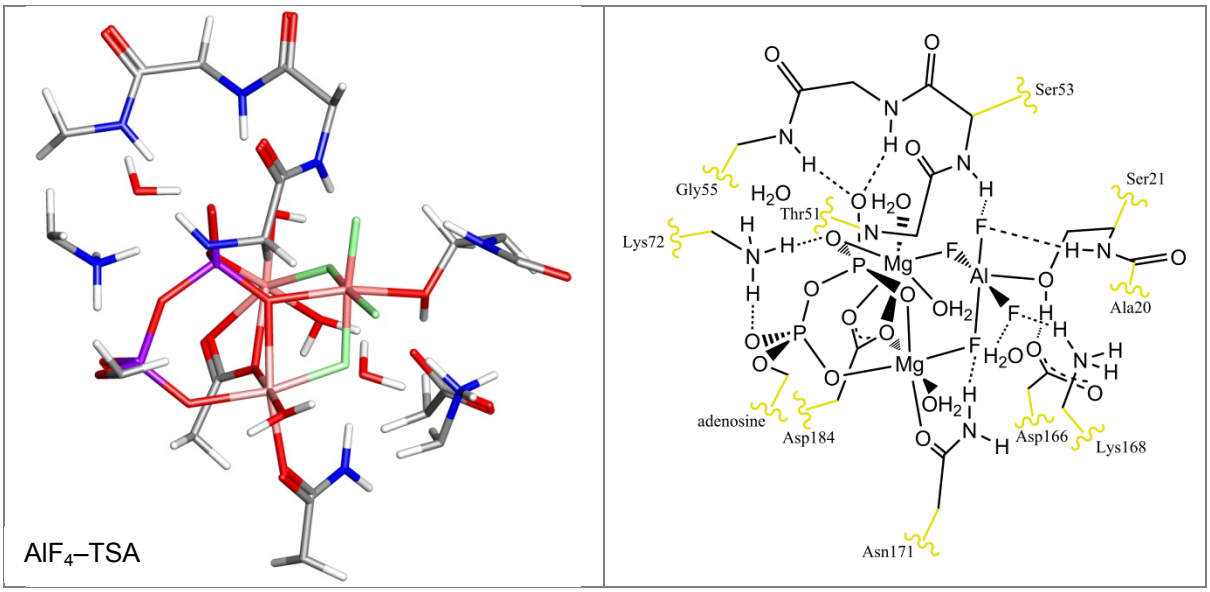
Table S3. 3D and 2D representations of the active site of each optimized geometry. Bonds in yellow denote the beginning of atoms that were constrained.






BeF3− TS
Ser53
Gly55
Thr51
Ser21
Lys72
Ala20
adenosine
Asp184
Asp166
Lys168
Asn171
BeF3− on Ser21
Ser53
Gly55
Thr51
Ser21
Lys72
Ala20
adenosine
Asp184
Asp166
Lys168
Asn171


MgF3–TSA
AlF3–TSA
Ser53
Gly55
Thr51
Lys72
Ser21
Ala20
adenosine
Asp184
Asp166
Lys168
Asn171
Mg
Al
F
P
O
N
H
H2O
OH2



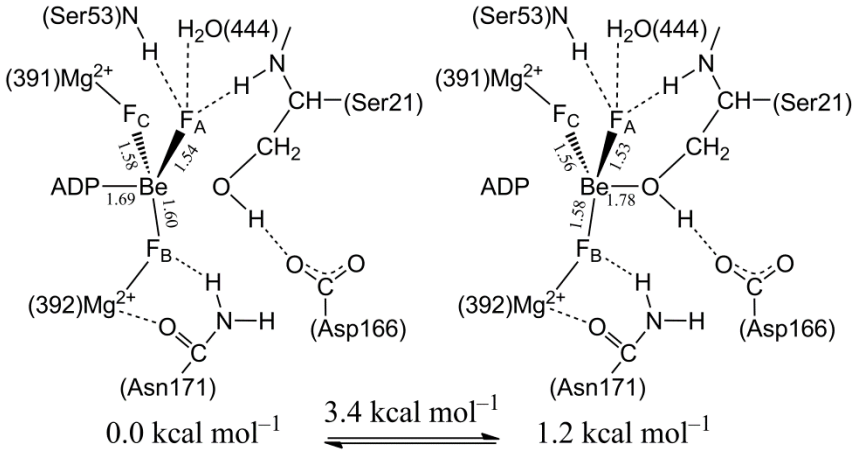


Figure S3. Computed structures of the tetrahedral reactant and product of BeF_3^- transfer in cAPK. A five-coordinate transition-state connects the two structures (with bond lengths in Å).

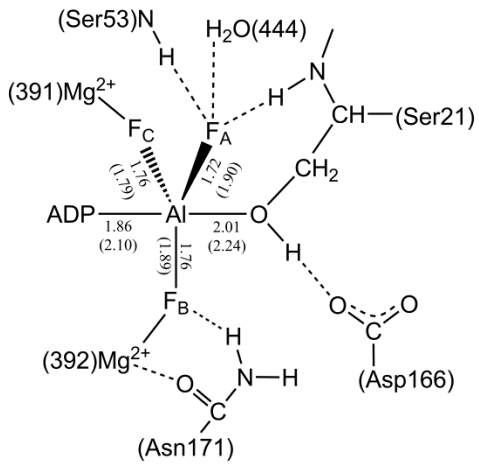


Figure S4. Computed structure of the active site in the AlF_3–TSA complex (with bond lengths in Å). Hydrogen bonds from the MgF_3–TSA X-ray crystal structure are in parenthesis.

Comparisons of other methods

The B3LYP/BS2 optimized geometries showed no significant geometric or energetic differences compared to the B3LYP/BS1 optimizations. From these results it appears that the 6-31G(d') basis sets was sufficient. Optimization using dispersion corrections also had little effect on the geometries and relative energies of the complexes. In the B3LYP-D/BS1 and ωB97xD/BS1 optimizations of the phosphoryl transfer transition-states, there was a second small imaginary frequency. This frequency corresponds to the movement of the hydrogen-bound water near Lys72. This pesky water moves during these other optimizations and slightly lower energy minima may be located (the location of this water does not have a significant effect on the relative energies of the sets of minima or their connecting TSs). It should be noted, however, that the choice of basis set or functional did not have any significant effect on the geometry within the cAPK active site.

Table S4. Energies. Absolute energies (Hartrees), relative energies (kcal mol^{-1}), and RMSD values (Å).

	optimized									single-point		
B3LYP/BS1	E	E_0	U	H	G	ΔE_{gas}	ΔG_{gas}	ΔG_{soln}	RMSD[a]	E	ΔE_{gas}	$\Delta\Delta E_{gas}$
PO_3^- on ADP	-10430.16343	-10429.36499	-10429.30162	-10429.30067	-10429.45639	0.0	0.0	0.0	-	-	-	-
PO_3^- TS	-10430.15332	-10429.35603	-10429.29345	-10429.29251	-10429.44618	6.3	6.4	5.8	-	-	-	-
PO_3^- on Ser21	-10430.15513	-10429.35742	-10429.29431	-10429.29337	-10429.44799	5.2	5.3	1.2	-	-	-	-
BeF_3^- on ADP	-10177.60028	-10176.80534	-10176.74119	-10176.74025	-10176.89752	0.0	0.0	0.0	-	-	-	-
BeF_3^- TS	-10177.59334	-10176.79929	-10176.73559	-10176.73465	-10176.89075	4.4	4.2	3.4	-	-	-	-
BeF_3^- on Ser21	-10177.59522	-10176.80053	-10176.73643	-10176.73549	-10176.89239	3.2	3.2	1.2	-	-	-	-
MgF_3–TSA	-10362.95150	-10362.15902	-10362.09426	-10362.09332	-10362.25158	-	-	-	-	-	-	-
AlF_3–TSA	-10405.07303	-10404.27907	-10404.21515	-10404.21420	-10404.37061	-	-	-	-	-	-	-
AlF_4–TSA	-10505.20058	-10504.40396	-10504.33854	-10504.33759	-10504.49741	-	-	-	-	-	-	-
B3LYP/BS2												
PO_3^- on ADP	-10430.51273	[b]	[b]	[b]	[b]	0.0	[b]	[b]	0.082	-10430.51011	0.0	-1.6
PO_3^- TS	[b]	[b]	[b]	[b]	[b]	[b]	[b]	[b]	[b]	-10430.49949	6.7	[b]
PO_3^- on Ser21	-10430.50445	[b]	[b]	[b]	[b]	5.2	[b]	[b]	0.087	-10430.50163	5.3	-1.8
BeF_3^- on ADP	-10177.95209	[b]	[b]	[b]	[b]	0.0	[b]	[b]	0.060	-10177.94944	0.0	-1.7
BeF_3^- TS	-10177.94445	[b]	[b]	[b]	[b]	4.8	[b]	[b]	0.056	-10177.94193	4.7	-1.6
BeF_3^- on Ser21	-10177.94726	[b]	[b]	[b]	[b]	3.0	[b]	[b]	0.111	-10177.94440	3.2	-1.8
MgF_3–TSA	-10363.30528	[b]	[b]	[b]	[b]	-	-	[b]	0.091	-10363.30022	-	-3.2
AlF_3–TSA	-10405.41873	[b]	[b]	[b]	[b]	-	-	[b]	0.056	-10405.41623	-	-1.6
AlF_4–TSA	-10505.56172	[b]	[b]	[b]	[b]	-	-	[b]	0.079	-10505.55864	-	-1.9
B3LYP-D/BS1												
PO_3^- on ADP	-10431.08608	-10430.28709	-10430.22404	-10430.22309	-10430.37770	0.0	0.0	[b]	0.076	-10431.08371	0.0	-1.5
PO_3^- TS[c]	-10431.07649	-10430.27881	-10430.21730	-10430.21636	-10430.36697	6.0	6.7	[b]	0.078	-10431.07440	5.8	-1.3
PO_3^- on Ser21	-10431.07753	-10430.27909	-10430.21636	-10430.21542	-10430.36892	5.4	5.5	[b]	0.064	-10431.07541	5.2	-1.3
BeF_3^- on ADP	-10178.50677	-10177.71153	-10177.64750	-10177.64655	-10177.80392	0.0	0.0	[b]	0.087	-10178.50443	0.0	-1.5
BeF_3^- TS	[b]	[b]	[b]	[b]	[b]	[b]	[b]	[b]	[b]	-10178.49810	4.0	[b]
BeF_3^- on Ser21	-10178.50600	-10177.71014	-10177.64659	-10177.64565	-10177.80100	0.5	1.8	[b]	0.271	-10178.49995	2.8	-3.8
MgF_3–TSA	-10363.86639	-10363.07315	-10363.00879	-10363.00785	-10363.16472	-	-	[b]	0.075	-10363.86423	-	-1.4
AlF_3–TSA	-10405.98692	-10405.19231	-10405.12873	-10405.12779	-10405.28321	-	-	[b]	0.057	-10405.98496	-	-1.2
AlF_4–TSA	-10506.12115	-10505.32368	-10505.25863	-10505.25769	-10505.41623	-	-	[b]	0.082	-10506.11889	-	-1.4
ωB97xD/BS1												
PO_3^- on ADP	-10427.64522	-10426.83568	-10426.77316	-10426.77222	-10426.92596	0.0	0.0	[b]	0.090	-10427.64115	0.0	-2.5
PO3– TS[c]	-10427.63406	-10426.82591	-10426.76487	-10426.76392	-10426.91370	7.0	7.7	[b]	0.071	-10427.63001	7.0	-2.5
PO_3^- on Ser21	-10427.63730	-10426.82923	-10426.76663	-10426.76568	-10426.91953	5.0	4.0	[b]	0.072	-10427.63347	4.8	-2.4
BeF_3^- on ADP	-10175.07420	-10174.26761	-10174.20451	-10174.20356	-10174.35818	0.0	0.0	[b]	0.261	-10175.06722	0.0	-4.4
BeF_3^- TS	-10175.06586	[b]	[b]	[b]	[b]	5.2	[b]	[b]	0.065	-10175.06212	3.2	-2.4
BeF_3^- on Ser21	-10175.06669	-10174.262064	-10174.198352	-10174.197408	-10174.35447	4.7	2.3	[b]	0.076	-10175.06285	2.7	-2.4
MgF_3–TSA	-10360.41335	-10359.60990	-10359.54591	-10359.54496	-10359.70147	-	-	[b]	0.086	-10360.40961	-	-2.4
AlF_3–TSA	-10402.53552	-10401.73080	-10401.66767	-10401.66672	-10401.82161	-	-	[b]	0.058	-10402.53203	-	-2.2
AlF_4–TSA	-10502.64319	-10501.83548	-10501.77108	-10501.77013	-10501.92697	-	-	[b]	0.095	-10502.63928	-	-2.5

[a]RMSD of non-constrained atoms compared to B3LYP/6-31G(d') geometry; [b]Calculation was not performed; [c]Includes a second imaginary frequency

Table S5. Computed bond lengths (Å) and angles (°) of gas-phase optimized geometries.

	B3LYP/ BS1	B3LYP/ BS2	B3LYP-D/ BS1	ωB97xD/ BS1
PO_3^- on ADP				
$P–O_{ADP}$	1.78	1.77	1.78	1.76
$P–O_A$	1.52	1.52	1.52	1.51
$P–O_B$	1.54	1.54	1.54	1.54
$P–O_C$	1.53	1.53	1.53	1.52
$P–O_{Ser21}$	2.77	2.80	2.73	2.78
$O_{ADP}–O_{Ser21}$	4.52	4.55	4.48	4.52
$<O_{ADP}–P–O_{Ser21}$	168.0	168.7	168.2	168.5
PO_3^- TS				
$P–O_{ADP}$	2.41	[a]	2.38	2.63
$P–O_A$	1.51	[a]	1.51	1.50
$P–O_B$	1.54	[a]	1.54	1.53
$P–O_C$	1.52	[a]	1.52	1.51
$P–O_{Ser21}$	1.98	[a]	1.97	1.98
$O_{ADP}–O_{Ser21}$	4.38	[a]	4.33	4.32
$<O_{ADP}–P–O_{Ser21}$	170.3	[a]	170.6	170.7
PO_3^- on Ser21				
$P–O_{ADP}$	2.75	2.77	2.71	2.75
$P–O_A$	1.52	1.53	1.52	1.52
$P–O_B$	1.55	1.55	1.55	1.54
$P–O_C$	1.53	1.53	1.53	1.52
$P–O_{Ser21}$	1.75	1.75	1.75	1.73
$O_{ADP}–O_{Ser21}$	4.49	4.52	4.45	4.47
$<O_{ADP}–P–O_{Ser21}$	171.1	172.1	171.4	171.7
BeF_3^- on ADP				
$Be–O_{ADP}$	1.69	1.69	1.69	1.71
$Be–F_A$	1.54	1.55	1.54	1.55
$Be–F_B$	1.60	1.60	1.60	1.61
$Be–F_C$	1.58	1.58	1.58	1.58
$Be–O_{Ser21}$	2.83	2.84	2.79	2.77
$O_{ADP}–O_{Ser21}$	4.49	4.51	4.46	4.46
$<O_{ADP}–Be–O_{Ser21}$	166.9	167.3	167.2	167.9
BeF_3^- TS				
$Be–O_{ADP}$	2.18	2.19	[a]	2.17
$Be–F_A$	1.53	1.54	[a]	1.54
$Be–F_B$	1.58	1.57	[a]	1.59
$Be–F_C$	1.57	1.56	[a]	1.57
$Be–O_{Ser21}$	2.05	2.07	[a]	2.03
$O_{ADP}–O_{Ser21}$	4.21	4.24	[a]	4.18
$<O_{ADP}–Be–O_{Ser21}$	170.7	171.1	[a]	170.8
BeF_3^- on Ser21				
$Be–O_{ADP}$	2.61	2.66	2.59	2.52
$Be–F_A$	1.53	1.54	1.54	1.54
$Be–F_B$	1.58	1.58	1.58	1.59
$Be–F_C$	1.53	1.56	1.56	1.57
$Be–O_{Ser21}$	1.78	1.76	1.77	1.81
$O_{ADP}–O_{Ser21}$	4.37	4.42	4.34	4.32
$<O_{ADP}–Be–O_{Ser21}$	171.6	172.4	172.1	171.6

[a]Calculation was not performed

Table S5 (cont.). Computed bond lengths (Å) and angles (°) of gas-phase optimized geometries.

	B3LYP/ BS1	B3LYP/ BS2	B3LYP-D/ BS1	ωB97xD/ BS1
MgF_3–TSA				
Mg–O_{ADP}	2.05	2.05	2.05	2.05
Mg–F_A	1.90	1.91	1.90	1.90
Mg–F_B	1.93	1.93	1.93	1.93
Mg–F_C	1.91	1.91	1.90	1.91
Mg–O_{Ser21}	2.14	2.15	2.13	2.14
O_{ADP}–O_{Ser21}	4.16	4.16	4.14	4.15
<O_{ADP}–Mg–O_{Ser21}	164.6	165.2	164.6	164.0
AlF_3–TSA				
Al–O_{ADP}	1.86	1.86	1.85	1.85
Al–F_A	1.72	1.73	1.72	1.72
Al–F_B	1.76	1.76	1.76	1.76
Al–F_C	1.76	1.75	1.75	1.75
Al–O_{Ser21}	2.01	2.01	2.00	2.01
O_{ADP}–O_{Ser21}	3.85	3.85	3.84	3.85
<O_{ADP}–Al–O_{Ser21}	169.3	169.7	169.5	169.8
AlF_4–TSA				
Al–O_{ADP}	1.96	1.96	1.95	1.95
Al–F_A	1.75	1.75	1.75	1.74
Al–F_B	1.81	1.82	1.81	1.80
Al–F_C	1.86	1.86	1.86	1.86
Al–F_D	1.83	1.83	1.83	1.83
Al–O_{Ser21}	2.04	2.04	2.02	2.04
O_{ADP}–O_{Ser21}	3.95	3.96	3.93	3.95
<O_{ADP}–Al–O_{Ser21}	163.8	163.7	163.8	163.7

[a]Calculation was not performed

Solvation effects

Solvation stabilizes the relative energies of the PO_3^- and BeF_3^- conformers when compared to gas phase (Table S6). In particular, the relative energy of the CPCM//B3LYP/BS1 optimized S21-bound species is decreased by 4.1 and 2.0 kcal mol^{-1} for PO_3^- and BeF_3^-, respectively, while the energy of activation for each is reduced by a smaller magnitude. Solvation has little effect, however, on the computed ^{19}F NMR chemical shifts of the TSAs (Table S7). The difference in chemical shift for each fluoride is less than one ppm.

The CPCM-B3LYP/BS1 optimized PO_3^- complexes were also very similar geometrically to the gas-phase optimizations. The distance between the axial oxygen atoms in the phosphoryl transfer transition state is shortened (4.32 Å) compared to the ADP- and Ser21-bound complexes (each minimum had a distance of 4.52 Å). In the CPCM-B3LYP/BS1 geometry, the P–O_{axial} bonds of the transition state are more equidistant (2.23 and 2.10 Å) than those of the B3LYP/BS1 geometry (2.41 and 1.98 Å). The ΔE_{SCRF} of the CPCM-B3LYP/BS1 complex is only 0.5

kcal mol^{-1} lower in energy than the CPCM//B3LYP/BS1 complex, and the ΔG_{soln} is 1.4 kcal mol^{-1} lower, suggesting that the energy of the TS is not highly dependent on this distance (a somewhat surprising result!).

Table S6. Gas-phase and solution-phase (CPCM) relative energies (in kcal mol^{-1}) for PO_3^- and BeF_3^- complexes.

species	ΔG_{gas} B3LYP/BS1	ΔG_{soln} CPCM//B3LYP/BS1	ΔE_{SCRF} CPCM-B3LYP/BS1	ΔG_{soln} CPCM-B3LYP/BS1
PO_3^- on ADP	0.0	0.0	0.0	0.0
PO_3^- TS	6.4	5.8	5.3	4.4
PO_3^- on S21	5.3	1.2	0.1	0.4
BeF_3^- on ADP	0.0	0.0	[a]	[a]
BeF_3^- TS	4.2	3.4	[a]	[a]
BeF_3^- on S21	3.2	1.2	[a]	[a]

[a]Calculation was not performed

Table S7. Gas-phase and solution-phase (CPCM) computed ^{19}F NMR chemical shifts (in ppm) for TSA complexes.

TSA	Fx	gas	CPCM	difference
MgF_3^-	F_A	-167.7	-168.5	0.8
	F_B	-195.5	-195.2	-0.3
	F_C	-203.2	-203.4	0.2
AlF_3	F_A	-169.4	-170.2	0.8
	F_B	-176.3	-175.7	-0.6
	F_C	-176.1	-176.2	0.1
AlF_4^-	F_A	-170.1	-170.6	0.5
	F_B	-157.8	-157.9	0.1
	F_C	-165.3	-164.7	-0.6
	F_D	-181.7	-181.7	0.0

Table S8. Computed bond lengths (Å) of solution-phase (CPCM) optimized PO_3^- geometries.

	PO_3^- on ADP	PO_3^- TS	PO_3^- on Ser21
$P–O_{ADP}$	1.77	2.23	2.81
$P–O_A$	1.52	1.52	1.53
$P–O_B$	1.54	1.53	1.54
$P–O_C$	1.53	1.52	1.53
$P–O_{Ser21}$	2.78	2.10	1.73
$O_{ADP}–O_{Ser21}$	4.52	4.32	4.52
$<O_{ADP}–P–O_{Ser21}$	168.2	170.5	171.2

BeF_3^- ^{19}F NMR spectra for both ground-state analogues

The identity of the species that produced the experimental BeF_3^- ^{19}F NMR spectrum (Figure 4 of the main text) has not been resolved. The computationally-derived chemical shifts for the ADP-bound and Ser21-bound species (Figure S5) are not significantly different from one another, and therefore cannot identify which isomer was present. The lower energy isomer (ADP-bound BeF_3^-) was used in Figure 5 for comparison to the MgF_3–TSA spectrum.

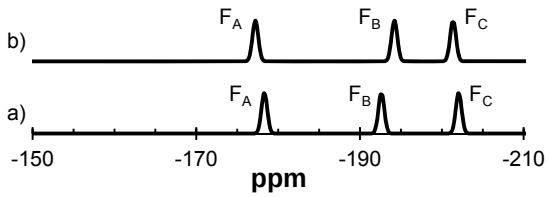


Figure S5. Computed ^{19}F NMR spectra and chemical shifts for a) BeF_3^- bound to ADP (-178.3, -192.6, -202.1 ppm), b) BeF_3^- bound to Ser21 (-177.2, -194.2, -201.4 ppm).

Derived APT charges

The optimized geometries of the transition-state analogues show that MgF_3^-, AlF_3, and AlF_4^- are good geometric mimics of the planar phosphoryl transfer transition-state. Analysis of the charges of individual atoms is also required to demonstrate that each analogue is also a good mimic of the electronic character of the five-coordinate phosphoryl species. Comparisons of atomic charge were performed using an atomic polar tensor (APT) charge derived from the Mulliken charges computed for each atom during the gas phase geometry optimization. Mulliken charges have been shown to be strongly dependent on basis set, but the computation of the more accurate APT charges[18, 19] is not implemented for systems with frozen atoms. A linear relationship between Mulliken and APT charges was established using simple PO_x, MgF_x, AlF_x, and BeF_x complexes (also computed in the gas phase), and that relationship was used to derive APT charges for the atoms of the large cAPK system (Figure S6).

Table S9. Calculated charges for simple complexes.

		X		Y		H	
species	atom	Mulliken	APT	Mulliken	APT	Mulliken	APT
$H_3PO_3^{2+}$	OH	1.3598	2.2960	-0.3738	-0.7235	0.5872	0.6248
	OH			-0.3738	-0.7235	0.5872	0.6248
	OH			-0.3738	-0.7235	0.5872	0.6248
$H_2PO_3^{+}$	OH	1.1236	1.8761	-0.4600	-0.7033	0.5170	0.4922
	OH			-0.4600	-0.7033	0.5171	0.4922
	O			-0.2378	-0.4540	–	–
HPO_3	OH	0.9511	1.6297	-0.5639	-0.7264	0.4393	0.3434
	O			-0.3986	-0.6036	–	–
	O			-0.4279	-0.6431	–	–
PO_3^{-}	O	0.7566	1.4210	-0.5855	-0.8070	–	–
	O			-0.5855	-0.8070	–	–
	O			-0.5855	-0.8070	–	–
BeF^{+}		1.0581	1.4936	-0.0581	-0.4936	–	–
BeF_2		0.5292	1.1536	-0.2646	-0.5768	–	–
				-0.2646	-0.5768	–	–
BeF_3^{-}		0.2587	1.0058	-0.4196	-0.6685	–	–
				-0.4196	-0.6686	–	–
				-0.4196	-0.6686	–	–
BeF_4^{2-}		0.1972	0.9829	-0.5493	-0.7457	–	–
				-0.5493	-0.7457	–	–
				-0.5493	-0.7457	–	–
				-0.5493	-0.7457	–	–
MgF^{+}		1.3910	1.5136	-0.3910	-0.5136	–	–
MgF_2		0.9531	1.2573	-0.4765	-0.6287	–	–
				-0.4766	-0.6287	–	–
MgF_3^{-}		0.6267	1.0581	-0.5422	-0.6861	–	–
				-0.5423	-0.6860	–	–
				-0.5422	-0.6860	–	–
MgF_4^{2-}		0.3711	0.9048	-0.5928	-0.7262	–	–
				-0.5928	-0.7262	–	–
				-0.5928	-0.7262	–	–
				-0.5928	-0.7262	–	–
MgF_5^{3-}		0.1312	0.6635	-0.6225	-0.7304	–	–
				-0.6226	-0.7298	–	–
				-0.6226	-0.7298	–	–
				-0.6317	-0.7367	–	–
				-0.6317	-0.7367	–	–
MgF_6^{4-}		0.0378	0.6121	-0.6732	-0.7690	–	–
				-0.6716	-0.7670	–	–
				-0.6732	-0.7690	–	–
				-0.6740	-0.7699	–	–
				-0.6718	-0.7673	–	–
				-0.6740	-0.7699	–	–
				-0.5422	-0.6860	–	–
AlF^{2+}		2.0566	2.1406	-0.0566	-0.1406	–	–
AlF_2^{+}		1.4524	1.8593	-0.2262	-0.4296	–	–
				-0.2262	-0.4296	–	–
AlF_3		1.1376	1.7237	-0.3792	-0.5745	–	–
				-0.3792	-0.5746	–	–
				-0.3792	-0.5746	–	–
AlF_4^{-}		0.9238	1.7029	-0.4810	-0.6757	–	–
				-0.4810	-0.6757	–	–
				-0.4810	-0.6757	–	–
				-0.4810	-0.6757	–	–
AlF_5^{2-}		0.8017	1.6525	-0.5523	-0.7277	–	–
				-0.5523	-0.7274	–	–
				-0.5522	-0.7274	–	–
				-0.5724	-0.7350	–	–
				-0.5724	-0.7350	–	–
AlF_6^{3-}		0.7386	1.6076	-0.6231	-0.7682	–	–
				-0.6231	-0.7677	–	–
				-0.6231	-0.7682	–	–
				-0.6231	-0.7679	–	–
				-0.6231	-0.7677	–	–
				-0.6231	-0.7679	–	–

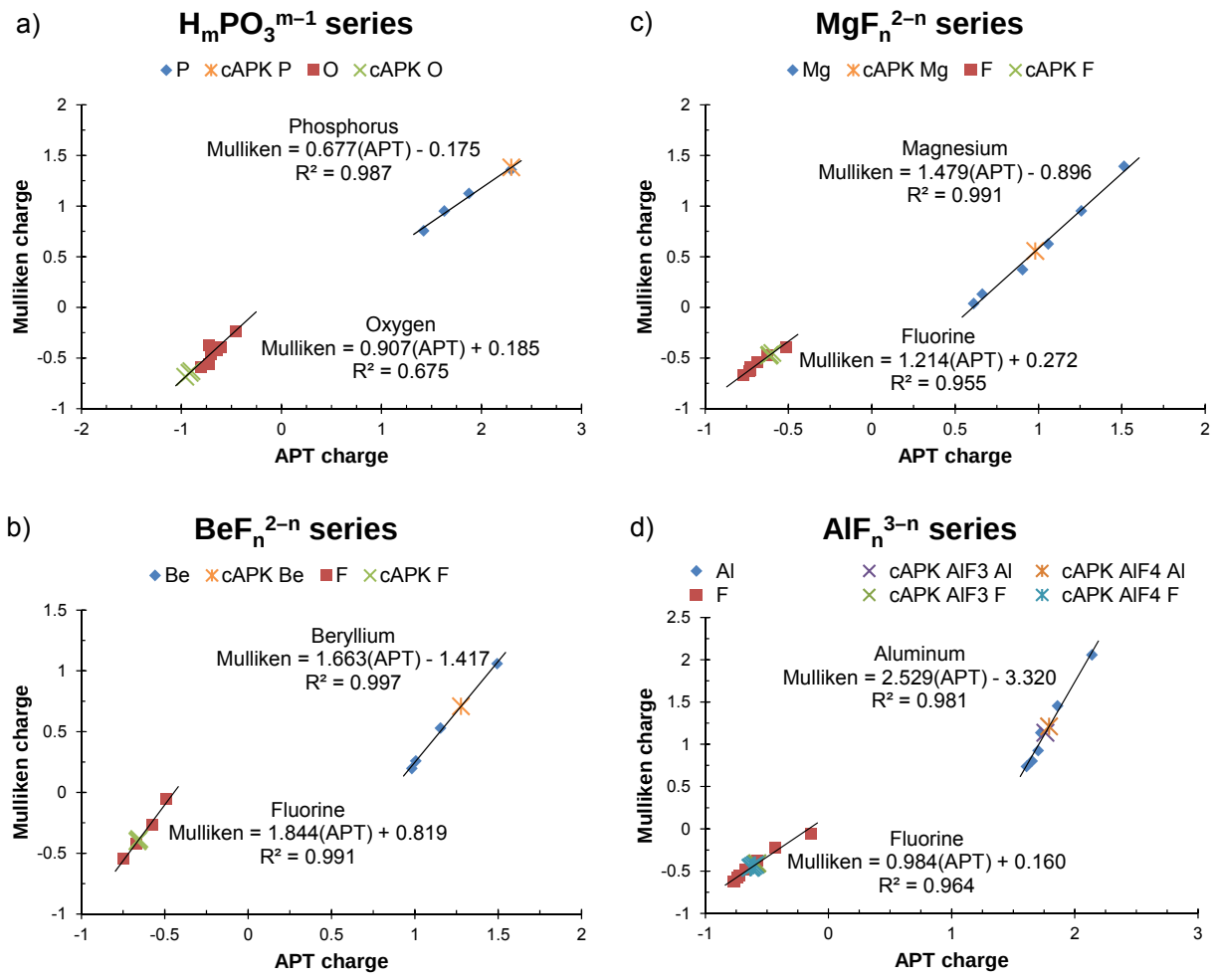


Figure S6. Computed Mulliken charges vs. APT charges for a) $H_mPO_3^{m-1}$ series, b) BeF_n^{2-n} series, c) MgF_n^{2-n} series, d) AlF_n^{3-n} series. Linear regressions were performed for each element. The charges of each five-coordinate cAPK species (six-coordinate in the case of AlF_4) is also plotted.

In the computed PO_3^- transition-state, the phosphorus atom has a very positive charge close to +2.3, while each of the oxygen atoms is nearly –1 (Table S10). None of the analogues exhibit such large magnitudes in its charges, but each metal atom is distinctly positive and each fluoride is negative. On average, the analogue contains about 60% of the charge of PO_3 and the distribution of the charge is similar. Derived APT charges were also calculated (Table S11) in the same manner for β-phosphoglucomutase (β-PGM), another phosphoryl transfer enzyme that has been demonstrated to form the analogous ground-state and transition-state analogues.[20, 21] The derived APT charges for β-PGM are very similar in magnitude to those of cAPK. In both cases, the phosphorus of the PO_3 species is the most positive of the X atoms, while the magnesium of the MgF_3 species is the least positive. Trends in the other atoms are also similar.

Table S10. Derived APT charges for five-coordinate (six-coordinate for AlF_4^-) cAPK species.

species	X	Y_A	Y_B	Y_C	Y_D
TS PO_3^-	2.2995	-0.9165	-0.9601	-0.8985	–
TS BeF_3^-	1.2773	-0.6589	-0.6633	-0.6525	–
MgF_3^-	0.9815	-0.6160	-0.6101	-0.5959	–
AlF_3	1.7619	-0.5840	-0.5926	-0.5769	–
AlF_4^-	1.7912	-0.5955	-0.6337	-0.6239	-0.6098

Table S11. Derived APT charges for five-coordinate (six-coordinate for AlF_4^-) β-PGM species.

species	X	Y	Y	Y	Y
TS PO_3^-	2.1118	-0.9418	-0.9315	-0.9243	–
TS BeF_3^-	1.2031	-0.6633	-0.6567	-0.6623	–
MgF_3^-	0.9745	-0.6248	-0.6026	-0.6113	–
AlF_3	1.7286	-0.6172	-0.5961	-0.5984	–
AlF_4^-	1.7357	-0.6327	-0.6160	-0.6405	-0.6376

Table S12. Computed Mulliken and derived APT charges for functionals with BS1.[a]

	B3LYP		B3LYP-D	ωB97xD
	Mulliken	APT	Mulliken	Mulliken
PO_3^- on ADP				
P	1.4008	2.3269	1.4123	1.3865
O_{ADP}	-0.7354	-1.0150	-0.7378	-0.7429
O_A	-0.6466	-0.9167	-0.6506	-0.6532
O_B	-0.6794	-0.9530	-0.6817	-0.6898
O_C	-0.6461	-0.9160	-0.6453	-0.6543
O_{Ser21}	-0.6233	-0.8910	-0.6245	-0.6299
PO_3^- TS				
P	1.3817	2.2995	1.3961	1.3749
O_{ADP}	-0.7025	-0.9785	-0.7044	-0.7171
O_A	-0.6463	-0.9165	-0.6505	-0.6494
O_B	-0.6858	-0.9601	-0.6901	-0.6940
O_C	-0.6300	-0.8985	-0.6314	-0.6386
O_{Ser21}	-0.6394	-0.9090	-0.6384	-0.6450
PO_3^- on Ser21				
P	1.3665	2.2768	1.3777	1.3570
O_{ADP}	-0.6656	-0.9375	-0.6682	-0.6750
O_A	-0.6683	-0.9404	-0.6703	-0.6737
O_B	-0.7202	-0.9981	-0.7222	-0.7311
O_C	-0.6525	-0.9233	-0.6524	-0.6638
O_{Ser21}	-0.6189	-0.8863	-0.6193	-0.6189
BeF_3^- on ADP				
Be	0.6749	1.2579	0.6781	0.7101
O_{ADP}	-0.6648	[b]	-0.6657	-0.6832
F_A	-0.4059	-0.6643	-0.4050	-0.4224
F_B	-0.4055	-0.6641	-0.4062	-0.4208
F_C	-0.3898	-0.6555	-0.3883	-0.4043
O_{Ser21}	-0.6157	[b]	-0.6171	-0.6241
BeF_3^- TS				
Be	0.7071	1.2773	[c]	[c]
O_{ADP}	-0.6889	[b]	[c]	[c]
F_A	-0.3959	-0.6589	[c]	[c]
F_B	-0.4042	-0.6633	[c]	[c]
F_C	-0.3843	-0.6525	[c]	[c]
O_{Ser21}	-0.6148	[b]	[c]	[c]

See next page for notes

Table S12 (cont.). Computed Mulliken and derived APT charges for functionals with BS1.[a]

	B3LYP		B3LYP-D	ωB97xD
	Mulliken	APT	Mulliken	Mulliken
BeF_3^- on Ser21				
Be	0.6483	1.2419	0.6528	0.6984
O_{ADP}	-0.6620	[b]	-0.6553	-0.6780
F_A	-0.3960	-0.6589	-0.3950	-0.4122
F_B	-0.4075	-0.6651	-0.4091	-0.4232
F_C	-0.3837	-0.6522	-0.3802	-0.4021
O_{Ser21}	-0.5988	[b]	-0.5975	-0.6197
MgF_3–TSA				
Mg	0.5557	0.9815	0.5564	0.5828
O_{ADP}	-0.7198	[b]	-0.7213	-0.7341
F_A	-0.4759	-0.6160	-0.4756	-0.4876
F_B	-0.4687	-0.6101	-0.4691	-0.4781
F_C	-0.4515	-0.5959	-0.4517	-0.4633
O_{Ser21}	-0.6407	[b]	-0.6427	-0.6530
AlF_3–TSA				
Al	1.1359	1.7619	1.1383	1.1623
O_{ADP}	-0.7418	[b]	-0.7424	-0.7558
F_A	-0.4147	-0.5840	-0.4149	-0.4274
F_B	-0.4231	-0.5926	-0.4239	-0.4334
F_C	-0.4076	-0.5769	-0.4070	-0.4192
O_{Ser21}	-0.6469	[b]	-0.6465	-0.6568
AlF_4–TSA				
Al	1.2100	1.7912	1.2133	1.2315
O_{ADP}	-0.7432	[b]	-0.7442	-0.7564
F_A	-0.4260	-0.5955	-0.4255	-0.4341
F_B	-0.4636	-0.6337	-0.4626	-0.4734
F_C	-0.4539	-0.6239	-0.4551	-0.4631
F_D	-0.4400	-0.6098	-0.4391	-0.4489
O_{Ser21}	-0.6418	[b]	-0.6426	-0.6516

[a]Charges from the B3LYP/BS2 optimizations are not comparable to those in the table due to the basis set dependency of Mulliken charges.
[b]Oxygen atoms were not included in the fluorine-containing series calculations
[c]Calculation was not performed

The derived APT charge of the phosphorus during the transition state is 2.2995, very similar to the phosphorus in $H_3PO_3^{2+}$ (2.2960), yet very different than the phosphorus in metaphosphate PO_3^- (1.4210). Evidence of the transition-state being more phosphorane-like is also seen in the distance between the oxygen of ADP and the Ser21 hydroxyl oxygen. For gas-phase optimization, the distance remains nearly the same in both the ADP-bound and Ser21-bound minima (4.52 and 4.49 Å, respectively). However, during the phosphoryl transfer transition state, this distance decreases to 4.38 Å, indicative of a phosphorane-like geometry and an associative process. Similar results were obtained for the solution-phase optimizations (see page S15).

Coordinates for optimized geometries

B3LYP/BS1 PO_3^- bound to ADP

H	-7.017091	7.152651	-2.634060
H	7.336002	7.876325	-0.678808
H	4.550783	7.487598	-0.641088
H	4.927791	8.539305	0.751132
H	1.659718	-2.552970	5.324853
H	2.089012	-2.402071	7.031248
H	-0.291201	-1.784973	6.358011
H	5.205714	-3.128939	2.081363
H	6.186651	-4.264429	3.012683
H	5.053282	-5.120660	5.250978
H	2.988941	-6.245225	5.995494
H	0.873341	-5.898437	4.669009
H	0.833234	-4.540327	2.880286
H	2.909346	-3.411293	1.980530
H	11.291691	1.088474	-5.403512
H	10.278818	1.836250	-2.711591
H	8.849257	0.575734	-4.394369
H	9.969418	-0.783342	-4.263561
H	9.394469	-1.159068	-1.988097
H	8.558817	0.391560	-1.860824
H	6.882648	-0.392052	-3.511336
H	7.707950	-1.951198	-3.594217
H	-4.976958	-4.878498	-4.646077
H	-5.739075	-3.746350	-2.025854
H	-6.106172	1.015341	-4.866067
H	-8.337298	2.193965	-3.429520
H	-6.946074	2.900840	-1.426547
H	-7.404614	1.195367	-1.434686
H	-5.109674	0.598124	-2.206410
H	-4.659209	2.304665	-2.145136
H	-5.126746	2.394372	0.248326
H	-5.744868	0.740140	0.227749
H	-6.633301	5.828015	-5.298519
H	-7.499028	7.718577	-4.236068
H	-9.351398	6.720918	-2.712634
H	-9.280852	6.181235	-4.392732
H	-8.096920	4.760864	-1.923784
H	-9.027353	4.044522	-3.242916
H	-3.767229	3.464967	-3.652025
H	-0.931560	3.005707	-4.553441
H	3.031360	-0.446408	-6.868951
H	2.957558	-1.859450	-5.063048
H	2.046898	-4.582572	-3.987488
H	2.703553	-5.670725	-2.071207
H	3.653888	-6.767909	-3.110270
H	0.007932	-6.557200	-3.239439
H	0.058894	-9.299368	-2.030394
H	-2.323889	-7.419440	-2.516263
H	-2.399186	-9.003523	-1.739108
H	0.286803	-8.630601	-0.132664
H	0.674382	-7.537366	2.064979
H	-0.992852	-5.812223	2.832873
H	-2.801370	-5.318559	1.626628
H	-3.247150	-6.276604	-0.660156
H	-4.264855	-6.565518	2.699496
H	-6.890452	-5.941990	1.378584
H	-5.357183	-5.515575	0.570029
H	-7.572553	-3.820781	1.594490
H	-6.319279	-2.470529	3.955198
H	-7.144295	-1.044524	1.362361
H	-5.005333	-1.632493	1.052608
H	-6.427795	1.027338	2.515824
H	-7.745499	0.284067	3.426955
H	-6.079647	0.118527	3.989531
H	-3.433510	9.592740	4.863749
H	-4.424165	7.603659	3.049612
H	-1.596741	7.914163	4.232820

H	-2.012260	6.941862	2.818277
H	-2.535611	8.930080	1.519419
H	-2.382372	9.967108	2.940704
H	-0.379221	10.184068	1.626782
H	0.048312	9.291321	3.089377
H	-0.310339	8.192151	0.318484
H	1.640183	6.244406	3.328404
H	0.759397	7.690548	3.692943
H	1.729001	5.465489	1.164452
H	0.915143	6.324489	-0.100365
H	3.663531	5.556770	-0.937545
H	2.443205	4.023339	-3.244024
H	0.539717	4.917086	-2.302052
H	2.214756	6.140736	-4.368983
H	2.810684	8.157651	-3.373028
H	4.719986	6.998933	-3.667678
H	12.007296	0.571796	-1.598579
H	-4.920859	9.371873	4.220254
H	6.189283	8.463717	-1.686219
H	10.837156	2.547258	-4.744565
H	1.663792	-1.197508	-7.430068
H	-4.569671	5.374303	3.152966
H	-3.438198	2.827273	6.553948
H	3.134865	-3.511154	-6.455441
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F    -0.593101  0.143028  0.268067
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B3LYP/BS1 BeF_3^- transfer transition-state

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F     0.148134  0.230532  3.067084
F     0.772211 -2.509227  0.983783
Mg    1.585151 -2.794285 -0.741596
Mg    0.599275  0.921054 -1.084589
Mg    0.195708 -0.746090  1.436225
    el energy= -10362.9515015
          zpe= -10362.159019
    th energy= -10362.094259
  th enthalpy= -10362.093315
  free energy= -10362.251575
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B3LYP/BS1 AlF_3-TSA

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H     7.244883  7.982436 -0.673422
H     4.464954  7.555917 -0.666516
H     4.809052  8.632857  0.714897
H     1.631440 -2.435696  5.408108
H     2.035975 -2.254207  7.117606
H    -0.343254 -1.679787  6.404222
H     5.227876 -3.009866  2.220291
H     6.211715 -4.118050  3.180989
H     5.060386 -4.957205  5.416604
H     3.001801 -6.099196  6.150457
H     0.899529 -5.800945  4.791379
H     0.864776 -4.469669  2.982485
H     2.937136 -3.325307  2.093511
H    11.355085  1.181816 -5.245404
H    10.296382  1.954611 -2.578297
H     8.906630  0.650161 -4.260940
H    10.043330 -0.691289 -4.095461
H     9.443298 -1.041784 -1.822451
H     8.585012  0.498854 -1.728985
H     6.941776 -0.331716 -3.389616
H     7.789251 -1.880375 -3.438708
H    -4.839533 -4.997357 -4.613635
H    -5.651769 -3.837602 -2.020534
H    -6.045788  0.876527 -4.935158
H    -8.311668  2.045026 -3.545501
H    -6.956980  2.800074 -1.535079
H    -7.392133  1.088499 -1.524124
H    -5.079222  0.511807 -2.256805
H    -4.652847  2.225107 -2.214762
H    -5.153381  2.343167  0.170762
H    -5.748638  0.680445  0.166472
H    -6.632519  5.674675 -5.445288
H    -7.537947  7.568363 -4.422228
H    -9.396699  6.567505 -2.908697
H    -9.296455  6.004475 -4.579599
H    -8.126294  4.636619 -2.074694
H    -9.029251  3.888405 -3.395226
H    -3.756746  3.375567 -3.726725
H    -0.903337  2.942399 -4.584087
H     3.136638 -0.488001 -6.796290
H     3.058011 -1.875558 -4.970902
H     2.170240 -4.595024 -3.867416
H     2.816085 -5.646091 -1.926840
H     3.794978 -6.745007 -2.937115
H     0.148540 -6.586504 -3.117183
H     0.220689 -9.309838 -1.867337
H    -2.180761 -7.470221 -2.412036
H    -2.244848 -9.043725 -1.612700
H     0.414192 -8.610469  0.023168
H     0.757571 -7.480153  2.209374
H    -0.943049 -5.767190  2.929857
H    -2.741893 -5.316110  1.692860
H    -3.144113 -6.313361 -0.585222
H    -4.202439 -6.567406  2.764682
H    -6.818452 -5.999426  1.400415
H    -5.280494 -5.563704  0.605848
H    -7.532153 -3.884914  1.576105
H    -6.328904 -2.483320  3.932914
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H	-7.138639	-1.106655	1.308769
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H	-7.785297	0.243369	3.345519
H	-6.124986	0.109020	3.932270
H	-3.619823	9.630542	4.701549
H	-4.559090	7.601818	2.904053
H	-1.752155	7.968466	4.119542
H	-2.135541	6.970060	2.714138
H	-2.668543	8.931774	1.379399
H	-2.548361	9.991373	2.787151
H	-0.531028	10.216816	1.496563
H	-0.110906	9.351412	2.977621
H	-0.417647	8.207227	0.218745
H	1.518935	6.330543	3.282335
H	0.613784	7.769545	3.613963
H	1.647149	5.521553	1.131434
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H	3.608055	5.608916	-0.946118
H	2.439534	4.025437	-3.245591
H	0.511690	4.906443	-2.341921
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H	2.752434	8.162110	-3.430609
H	4.681072	7.025677	-3.683104
H	12.026924	0.730437	-1.424220
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H	-4.675625	5.372406	3.038298
H	-3.555011	2.890936	6.490954
H	3.276299	-3.544698	-6.336392
H	-4.028060	-4.092194	4.673039
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H	-5.727528	-7.193047	3.015448
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C	1.735493	-1.712646	6.218982
C	5.405210	-3.383431	3.231053
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C	4.152467	-4.862903	4.836857
C	2.995532	-5.488021	5.256901
C	1.803813	-5.342224	4.538433
C	1.802713	-4.546547	3.422570
C	2.950300	-3.947511	2.989362
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C	8.851987	-0.325613	-2.371899
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C	-6.904808	-1.529073	-5.109672
C	-7.375570	-0.444572	-4.075136
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C	-6.765875	1.836983	-2.061910
C	-5.329094	1.473299	-1.811675
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C	-6.584116	3.209596	-4.153776
C	-6.536788	5.672944	-4.375812
C	-7.451172	6.700744	-3.770190
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C	2.466550	4.905195	-2.602633
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O	-4.566924	-1.657675	-3.651033
O	-8.222389	-0.724643	-3.154145
O	-5.625007	3.066323	-4.806661
O	-4.372757	6.391735	-4.776909
O	-0.984876	5.032166	-3.211057
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O	2.326247	-7.432683	-5.316536
O	2.313036	-8.549737	-1.972308
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O	-4.820852	-4.242116	3.198372
O	-5.162512	-1.243381	1.851621
O	-9.335254	-2.854683	2.824369
O	1.321450	4.946648	-1.832905
O	2.551719	7.426071	-2.799691
O	4.779574	5.262853	-2.603747
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H	4.155938	-0.966509	3.745550
H	6.160035	-2.643449	5.133423
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H	8.171131	-0.179519	0.983905
H	8.873950	-0.243497	2.593804
H	7.203015	-2.338068	-1.090514
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H	4.736929	-2.201702	-1.335157
H	4.915200	-1.183606	-2.616357
H	5.430778	-2.795946	-2.764972
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H	-2.807751	-3.262932	-2.885016
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H	-2.997262	-0.913188	-3.216935
H	1.696771	0.092084	-4.093659
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H	4.361352	-4.616324	-4.049311
H	2.530834	-4.874238	0.851491
H	1.277068	-5.408451	0.077072
H	-1.046388	-3.508763	-0.977446
H	-0.279026	-3.796171	-2.339127
H	-0.006224	2.912302	0.646753

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H    -0.255695  1.883094  2.653783
H    -1.535977  2.801421  2.633368
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C     5.817426 -2.227805  4.182952
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C    -3.537808 -3.658017 -2.167139
C    -3.514510 -2.820132 -0.887228
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C    -1.698622  0.711080 -3.202000
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O    -0.204891 -3.871648 -1.376696
O     0.287954  2.745214 -0.276295
O    -4.139348  0.062584  5.175366
O    -1.561095 -1.628579  1.886501
O    -0.631397  2.702963  2.290946
P     3.640454  1.173094 -2.025881
P     3.200254 -0.521062  0.483095
F    -0.794824  0.085640  0.159164
F     0.262733  0.025545  2.867408
F     0.696950 -2.420068  1.003654
Mg    1.557744 -2.916011 -0.739290
Mg    0.578635  0.900808 -1.146925
Al    0.180673 -0.776961  1.344571
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           zpe= -10404.279071
    th energy= -10404.215148
  th enthalpy= -10404.214203
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free energy= -10404.370605

B3LYP/BS1 AlF_4-TSA

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H	4.769265	8.648167	0.714873
H	1.728265	-2.499479	5.310451
H	2.155335	-2.336886	7.016340
H	-0.237219	-1.769184	6.343296
H	5.283534	-3.009638	2.066082
H	6.287693	-4.123378	2.998899
H	5.173000	-4.998254	5.239380
H	3.132182	-6.162934	5.987069
H	1.009326	-5.861370	4.661125
H	0.940873	-4.507608	2.869967
H	2.993288	-3.338507	1.967023
H	11.279222	1.316212	-5.429771
H	10.252834	2.048278	-2.738651
H	8.848164	0.756077	-4.418355
H	9.995619	-0.579853	-4.285703
H	9.429545	-0.962968	-2.009242
H	8.562806	0.570690	-1.884325
H	6.901961	-0.249631	-3.532491
H	7.758571	-1.791935	-3.612992
H	-4.865143	-4.976799	-4.652567
H	-5.648625	-3.855443	-2.033951
H	-6.113334	0.892622	-4.882613
H	-8.367076	2.028549	-3.446974
H	-6.989387	2.767032	-1.446051
H	-7.413384	1.052633	-1.450849
H	-5.107243	0.500465	-2.222754
H	-4.691314	2.215865	-2.164820
H	-5.159352	2.300466	0.228738
H	-5.743937	0.634059	0.211482
H	-6.737803	5.692869	-5.323491
H	-7.640998	7.567488	-4.263988
H	-9.472053	6.535391	-2.737731
H	-9.391483	5.994184	-4.416886
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H	0.260307	-9.290259	-2.031658
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H	-4.115357	-6.635699	2.695652
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O	-1.508183	-10.233418	-3.789659
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F    -0.771922 -0.179027 -0.052174
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F     0.546425 -2.350630  0.771223
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CPCM-B3LYP/BS1 PO3- bound to ADP
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CPCM-B3LYP/BS1 phosphoryl transfer transition-state
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CPCM-B3LYP/BS1 PO3- bound to Ser21
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B3LYP/BS2 BeF_3^- transfer transition-state

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O     2.047528 -4.688638 -0.021968
O    -0.217370 -3.824411 -1.324169
O     0.245045  2.785513 -0.289172
O    -4.051953 -0.064160  5.476347
O    -1.726712 -1.639476  1.884723
O    -0.469318  2.638966  2.368199
P     3.699000  1.159667 -2.118003
P     3.287661 -0.443449  0.427899
F    -0.686111  0.053372  0.233159
F     0.202820 -0.047642  2.709002
F     0.631509 -2.162876  0.992630
Mg    1.496511 -2.707905 -0.689945
Mg    0.644541  0.868892 -1.066080
Be    0.067308 -0.755066  1.353091
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B3LYP/BS2 BeF3- bound to Ser21
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H     4.832305  8.599071  0.787402
H     1.645655 -2.519374  5.354993
H     2.060611 -2.361332  7.064296
H    -0.320835 -1.770065  6.372348
H     5.221572 -3.063520  2.138990
H     6.207298 -4.187259  3.079449
H     5.066187 -5.051730  5.310669
H     3.008145 -6.196543  6.041644
H     0.899020 -5.873888  4.698858
H     0.858156 -4.519092  2.907640
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H	8.874665	0.668635	-4.315541
H	10.007887	-0.678503	-4.174141
H	9.419905	-1.056604	-1.902422
H	8.567244	0.485440	-1.783923
H	6.911704	-0.318133	-3.445562
H	7.753785	-1.868773	-3.519721
H	-4.891838	-4.929594	-4.661240
H	-5.685456	-3.801548	-2.048863
H	-6.080585	0.951818	-4.899395
H	-8.334510	2.109423	-3.481468
H	-6.965707	2.833899	-1.469357
H	-7.406419	1.123735	-1.478089
H	-5.099686	0.549196	-2.231702
H	-4.667470	2.260429	-2.169896
H	-5.153779	2.349038	0.219860
H	-5.754488	0.688425	0.197417
H	-6.654472	5.758057	-5.343732
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H	-2.758698	-5.337089	1.628224
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H	-4.217112	-6.597517	2.692219
H	-6.839110	-6.003435	1.350750
H	-5.304361	-5.562362	0.552937
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H	-6.457438	0.972118	2.479864
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H	2.949968	-0.141060	6.689196
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P     3.335273 -0.404361  0.443808
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O     0.113442 -0.341377  2.719640
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Mg    1.545352 -2.661275 -0.647793
Mg    0.626494  0.820375 -0.942265
P    -0.274788 -1.043037  1.426210
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  th enthalpy= -10430.215419
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B3LYP-D/BS1 BeF_3^- bound to ADP

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H     5.005516 -5.166175  5.277449
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H     0.820815 -5.907740  4.682562
H     0.797856 -4.548874  2.894111
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H     8.580045  0.317448 -1.822109
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O     1.915995  0.149702  0.466038
O     3.185139 -1.957925 -0.248652
O     4.125788 -0.507329  1.656695
O     4.526699  2.448920 -2.084111
O     4.869960 -4.096333 -0.381252
O     1.690493 -4.751943 -0.101922
O    -0.358209 -3.755950 -1.442938
O     0.307324  2.722610 -0.207087
O    -4.073903  0.057490  5.297209
O    -1.792192 -1.635210  1.855993
O    -0.287575  2.413342  2.418227
P     3.684183  1.075458 -2.136421
P     3.289358 -0.521633  0.404340
F    -0.729321  0.009750  0.266471
F     0.171127 -0.231500  2.721207
F     0.505469 -2.235173  0.959035
Mg    1.394433 -2.757601 -0.707725
Mg    0.659368  0.827586 -0.985603
Be   -0.226506 -0.941895  1.420455
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          zpe= -10177.710142
    th energy= -10177.646592
  th enthalpy= -10177.645648
  free energy= -10177.800995

B3LYP-D/BS1 MgF3-TSA
H    -7.058199  7.105487 -2.663161
H     7.279861  7.950279 -0.647134
H     4.497878  7.538118 -0.621167
H     4.860103  8.593163  0.772452
H     1.666134 -2.525563  5.334239
H     2.086912 -2.370832  7.042423
H    -0.295529 -1.773897  6.358979
H     5.230607 -3.072134  2.105947
H     6.217116 -4.199187  3.041616
H     5.081499 -5.064614  5.275242
H     3.023558 -6.206416  6.011192
H     0.910764 -5.877646  4.675676
H     0.866818 -4.520178  2.886556
H     2.937151 -3.373831  1.995417
H    11.312587  1.195300 -5.353787
H    10.282034  1.934907 -2.666323
H     8.870294  0.662155 -4.354927
H    10.001294 -0.687421 -4.219123
H     9.419878 -1.067651 -1.946064
H     8.570662  0.475901 -1.822600
H     6.908159 -0.322042 -3.480077
H     7.746926 -1.874182 -3.559172
H    -4.908313 -4.908345 -4.664341
H    -5.691050 -3.782264 -2.047575
H    -6.086168  0.975745 -4.890180
H    -8.333218  2.135746 -3.463327
H    -6.956512  2.854599 -1.454594
H    -7.400637  1.145324 -1.464373
H    -5.097491  0.567317 -2.226243
H    -4.661679  2.277599 -2.163363
H    -5.140118  2.363705  0.228084
H    -5.744193  0.704328  0.205170
H    -6.651960  5.783747 -5.325729
H    -7.538077  7.667105 -4.267301
H    -9.388434  6.654102 -2.751565
H    -9.306213  6.114791 -4.431251
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H    -9.039616  3.980454 -3.279986
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H	-3.773111	3.445159	-3.666666
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H	3.002192	-1.822670	-5.048160
H	2.109943	-4.553189	-3.975997
H	2.767661	-5.635140	-2.057045
H	3.731566	-6.724678	-3.091666
H	0.084518	-6.544809	-3.236255
H	0.153433	-9.286277	-2.026513
H	-2.243010	-7.426550	-2.522828
H	-2.308265	-9.011100	-1.745716
H	0.367644	-8.615342	-0.127952
H	0.736670	-7.518566	2.071120
H	-0.948276	-5.807413	2.831621
H	-2.755749	-5.329164	1.617622
H	-3.183733	-6.291262	-0.670862
H	-4.213224	-6.588253	2.684492
H	-6.838346	-5.987046	1.352336
H	-5.305304	-5.547851	0.550219
H	-7.539194	-3.871625	1.564964
H	-6.307369	-2.510528	3.930727
H	-7.133346	-1.091892	1.334155
H	-4.988240	-1.661890	1.033603
H	-6.439220	0.986094	2.490278
H	-7.754476	0.231884	3.395941
H	-6.089693	0.080459	3.965612
H	-3.527158	9.576744	4.849353
H	-4.493318	7.579131	3.031385
H	-1.673658	7.913603	4.226527
H	-2.074966	6.937633	2.810408
H	-2.609519	8.921187	1.508984
H	-2.471053	9.959674	2.930719
H	-0.464240	10.193304	1.625273
H	-0.035419	9.304399	3.089829
H	-0.373034	8.201850	0.317637
H	1.581022	6.271031	3.336158
H	0.686550	7.709758	3.696696
H	1.685583	5.492582	1.172743
H	0.869897	6.344513	-0.095671
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H	2.430615	4.055860	-3.232403
H	0.515687	4.933683	-2.298680
H	2.189124	6.171097	-4.358702
H	2.763815	8.193102	-3.360588
H	4.684039	7.050461	-3.646924
H	12.016356	0.685212	-1.545758
H	-5.009848	9.343267	4.199590
H	6.132524	8.527850	-1.659509
H	10.842992	2.650298	-4.697037
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H	-4.620485	5.348643	3.134521
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H	4.410591	5.575522	-4.615894
H	-5.739300	-7.209543	2.940029
H	-4.403678	-5.690994	-3.326081
H	-6.957661	-3.479289	-4.472896
H	4.026936	6.631017	2.024418
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H	-2.527613	-6.937805	6.842718
H	-8.585330	-2.227764	4.612862
H	-2.741686	4.063769	-6.498070
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H	8.872778	2.063447	1.832887
H	-1.512693	1.751837	4.659223
H	-1.648918	1.432008	6.401656
H	-4.733513	4.377516	5.961444
H	-5.770695	3.821739	4.623186
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H	-2.921796	6.516742	-2.330061
H	-3.136514	5.081677	-1.316903
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C	5.247706	4.951592	2.498251
C	3.943720	4.192359	2.618937
C	1.781117	-1.814819	6.154273
C	5.414967	-3.461163	3.109574
C	4.167111	-4.188550	3.549237
C	4.168916	-4.957229	4.705173
C	3.012502	-5.582355	5.126635
C	1.815161	-5.420005	4.421180
C	1.808253	-4.608273	3.316962
C	2.955064	-4.008987	2.882049
C	7.945847	1.524720	2.029593
C	10.696386	1.142512	-3.305996
C	9.599836	0.182820	-3.710867
C	8.827447	-0.340513	-2.479751
C	7.539864	-1.014373	-2.913867
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C	-6.775273	1.898253	-1.996969
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C	-6.546626	5.766049	-4.257301
C	-7.450052	6.789705	-3.628656
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C	-5.788788	-5.715425	1.520715
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C	-6.720449	0.135001	3.085909
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C	2.742685	6.193223	-3.419993
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C	-4.771745	4.164210	4.893203
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C	-2.464423	-2.957332	5.344814
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N	-6.856488	0.856664	-4.189350
N	-7.083002	4.518950	-3.754860
N	-4.628067	5.354981	-2.767264
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N	2.236075	-3.781589	-6.197559
N	2.301745	-5.551250	-4.118946
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N	-5.113598	-6.823266	2.204578
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N	-4.225793	8.854956	4.677513
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O	0.497408	-1.240837	6.418831
O	6.958611	2.165568	2.364508
O	12.351132	-0.490033	-3.088027
O	-4.609377	-1.584339	-3.656064
O	-8.255141	-0.639720	-3.112772
O	-5.652619	3.161243	-4.733942
O	-4.382500	6.479341	-4.667602
O	-0.987946	5.079721	-3.152306
O	-1.915502	2.320229	-7.063881
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O	2.237833	-7.370358	-5.467239
O	2.248761	-8.535591	-2.139485
O	-1.617613	-10.205592	-3.794541
O	-4.815348	-4.266306	3.157255
O	-5.153676	-1.245623	1.856347
O	-9.325497	-2.850229	2.844253
O	1.330193	4.962323	-1.796503
O	2.564874	7.449063	-2.738553
O	4.782877	5.271735	-2.594026
O	-3.578089	6.423578	5.944417
O	-3.511539	2.775006	3.354296
O	-1.628584	-2.692143	6.237138
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H	2.050457	2.762324	3.523550
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H	8.093947	-0.206515	0.825834
H	8.862884	-0.371264	2.403285
H	7.156459	-2.256944	-1.122381
H	6.534175	-0.595440	-1.033219
H	4.676124	-1.967906	-1.279342
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H	5.328373	-2.853463	-2.486705
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H	0.201608	-0.757573	-4.515844
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H	5.381000	-5.375041	-1.102346
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O    -0.433785  2.704458  2.395965
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P     3.247594 -0.467492  0.439215
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F     0.148227  0.188579  3.075934
F     0.725113 -2.531010  0.985743
Mg    1.536755 -2.798431 -0.739647
Mg    0.591076  0.902247 -1.069319
Mg    0.166941 -0.767181  1.437743
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          zpe= -10363.073147
    th energy= -10363.008789
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  free energy= -10363.164716

B3LYP-D/BS1 AlF3-TSA
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H     4.850021  8.614803  0.737935
H     1.620924 -2.447780  5.410032
H     2.023677 -2.270456  7.120388
H    -0.352167 -1.685388  6.404380
H     5.219693 -3.031731  2.226627
H     6.197644 -4.145296  3.187114
H     5.039660 -4.983110  5.419793
H     2.975413 -6.117873  6.148936
H     0.876358 -5.809133  4.787231
H     0.849629 -4.475050  2.980269
H     2.927888 -3.337741  2.096029
H    11.374706  1.146253 -5.223859
H    10.315212  1.919361 -2.557157
H     8.922685  0.623021 -4.243768
H    10.053723 -0.723247 -4.078622
H     9.448946 -1.074684 -1.807015
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B3LYP-D/BS1 AlF_4-TSA

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O	8.136529	-2.125144	3.792329
O	-2.467199	-2.601689	-0.391774
O	-4.679617	-2.265627	-0.469730
O	-0.749123	1.418495	-2.523463
O	1.887051	-2.724422	-2.827274
O	0.742908	-1.097344	-1.924344
O	2.212922	1.447528	-2.081700
O	4.207672	0.237218	-3.210694
O	4.129312	0.433151	-0.677161
O	1.888086	0.143163	0.485370
O	3.229106	-1.895586	-0.221568
O	4.098821	-0.426567	1.700156
O	4.506256	2.482809	-2.068888
O	4.780216	-4.525449	-1.207687
O	1.866168	-4.684843	-0.057473

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O    -1.795885 -1.628301  1.876536
O    -0.342281  2.459012  2.407543
P     3.688344  1.100229 -2.098350
P     3.288521 -0.476736  0.438239
F    -0.739615  0.014381  0.263850
F     0.151273 -0.179635  2.749016
F     0.515255 -2.229024  1.001425
Mg    1.436226 -2.664883 -0.664719
Mg    0.656108  0.848538 -0.983299
Be   -0.197288 -0.902439  1.437416
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H     4.883693  8.580289  0.769354
H     1.663489 -2.530114  5.332975
H     2.084970 -2.376212  7.041075
H    -0.296122 -1.773562  6.358010
H     5.226000 -3.085734  2.104053
H     6.209934 -4.215094  3.039667
H     5.072650 -5.077497  5.273595
H     3.012072 -6.214195  6.010069
H     0.899827 -5.880418  4.674926
H     0.858846 -4.523042  2.885665
H     2.931796 -3.381846  1.994001
H    11.316928  1.166042 -5.357324
H    10.288702  1.908454 -2.669742
H     8.873535  0.638965 -4.357933
H    10.001266 -0.713351 -4.222200
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H     8.573940  0.453720 -1.825530
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H     7.744140 -1.894540 -3.561679
H    -4.918674 -4.897945 -4.664070
H    -5.698164 -3.769692 -2.047283
H    -6.082222  0.988976 -4.890325
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H    -6.947314  2.870322 -1.454777
H    -7.395609  1.162134 -1.464283
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H    -5.739922  0.717281  0.204987
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H    -2.259110 -7.422410 -2.522799
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ωB97xD/BS1 AlF_3-TSA

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